

FILE 'HOME' ENTERED AT 13:37:20 ON 11 MAR 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 13:37:30 ON 11 MAR 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

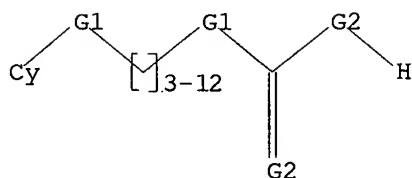
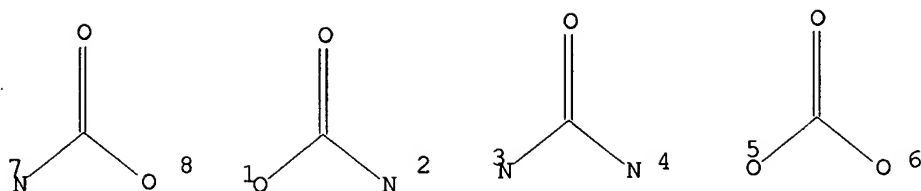
Uploading 10025947 rce first action.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 CH2,O,S,N, [01-02], [03-04], [05-06], [07-08]

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 13:38:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 561163 TO ITERATE

0.2% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

16 ANSWERS

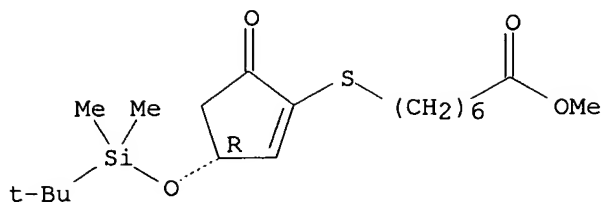
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 173898

L2 16 SEA SSS SAM L1

=> d scan

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Heptanoic acid, 7-[[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-oxo-1-cyclopenten-1-yl]thio]-, methyl ester, (R)- (9CI)
MF C19 H34 O4 S Si

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):16

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN L-Glutamine,

N-acetyl-L-.alpha.-aspartyl-L-phenylalanyl-L-.alpha.-glutamyl-

L-.alpha.-aspartyl-L-isoleucyl-L-prolyl-L-lysyl-L-.alpha.-glutamyl-L-

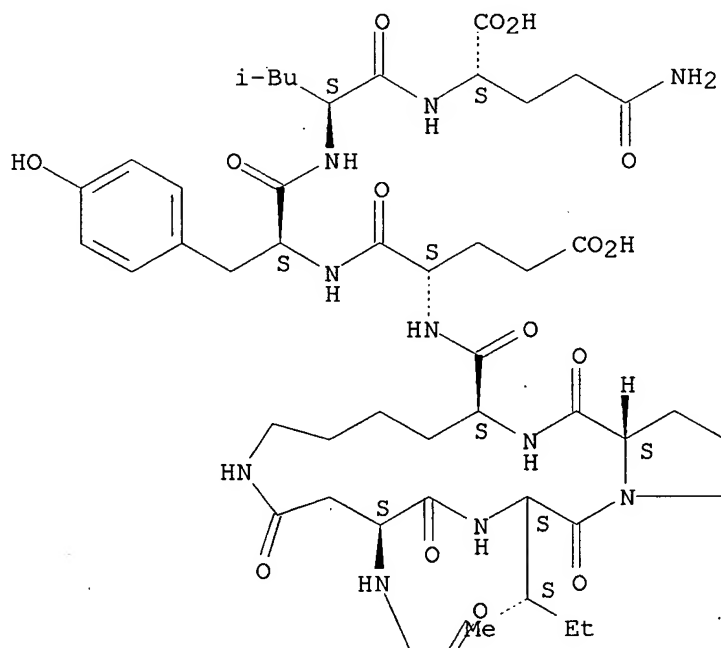
tyrosyl-L-leucyl-, cyclic (4.fwdarw.7)-peptide (9CI)

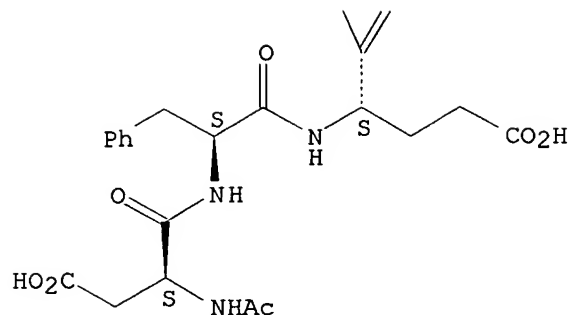
SQL 11

MF C66 H93 N13 O22

Absolute stereochemistry.

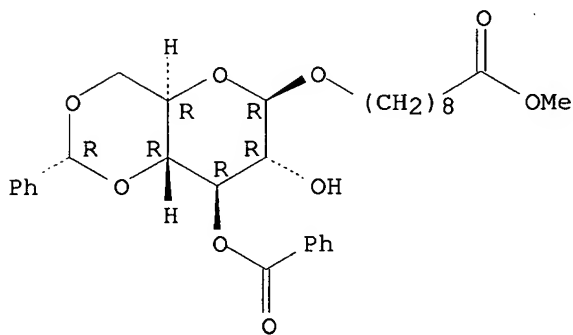
PAGE 1-A





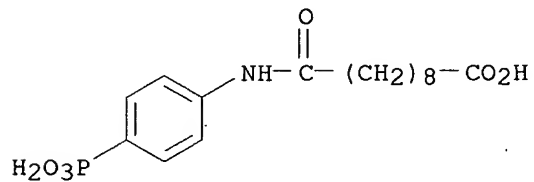
L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Nonanoic acid, 9-[[3-O-benzoyl-4,6-O-(phenylmethylene)-.beta.-D-glucopyranosyl]oxy]-, methyl ester, (R)- (9CI)
 MF C30 H38 O9

Absolute stereochemistry.



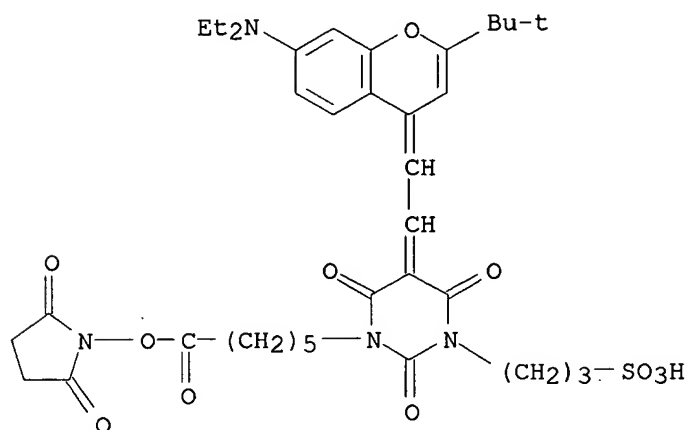
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Decanoic acid, 10-oxo-10-[(4-phosphonophenyl)amino]- (9CI)
 MF C16 H24 N O6 P



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

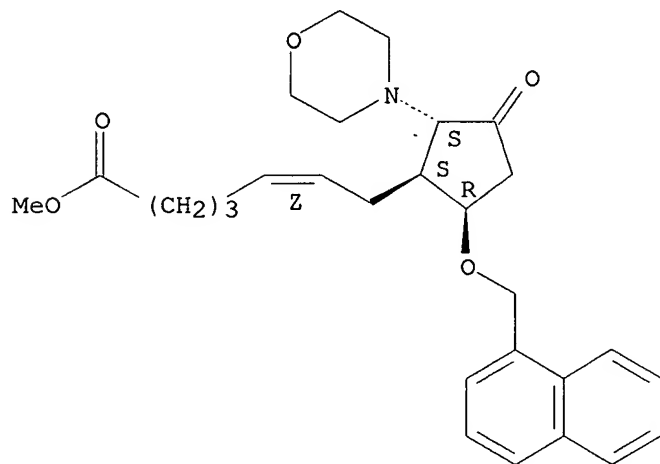
L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1(2H)-Pyrimidinepropanesulfonic acid, 5-[[7-(diethylamino)-2-(1,1-dimethylethyl)-4H-1-benzopyran-4-ylidene]ethylidene]-3-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]tetrahydro-2,4,6-trioxo-, sodium salt (9CI)
 MF C36 H46 N4 O11 S . Na

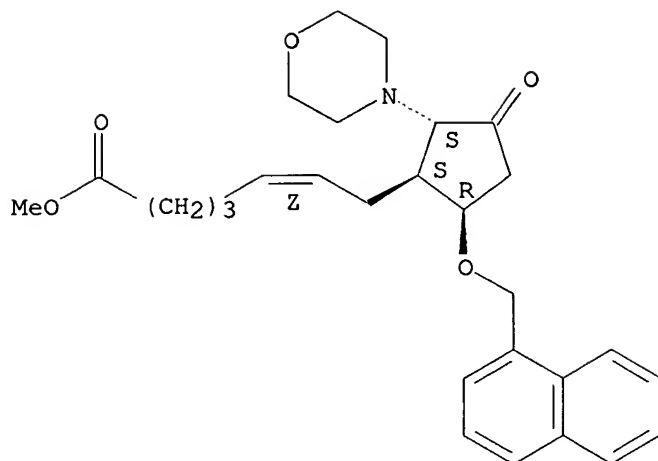


● Na

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 5-Heptenoic acid, 7-[2-(4-morpholinyl)-5-(1-naphthalenylmethoxy)-3-oxocyclopentyl]-, methyl ester, [1.alpha.(Z),2.beta.,5.alpha.]- (9CI)
 MF C28 H35 N O5

Relative stereochemistry.
 Double bond geometry as shown.



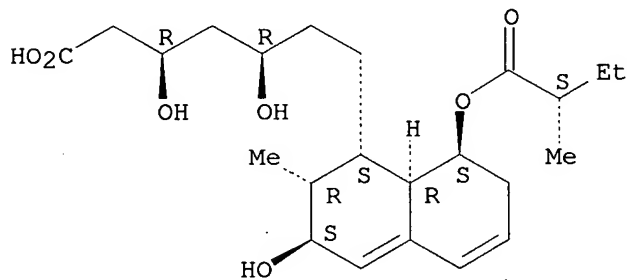


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

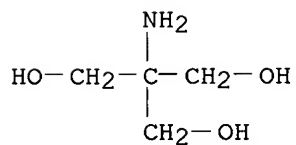
L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Naphthaleneheptanoic acid, 1,2,6,7,8,8a-hexahydro-.beta.,.delta.,6-
 trihydroxy-2-methyl-8-(2-methyl-1-oxobutoxy)-, [1S-
 [1.alpha.(.beta.S*,.delta.S*),2.alpha.,6.beta.,8.beta.(R*),8a.alpha.]]-,
 compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI)
 MF C23 H36 O7 . C4 H11 N O3

CM 1

Absolute stereochemistry.



CM 2



L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN L-Cysteinamide,

D-phenylalanyl-L-cysteiny-L-tyrosyl-L-tryptophyl-N6-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-lysyl-L-threonyl-N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)propyl]-, cyclic (2.fwdarw.7)-disulfide (9CI)

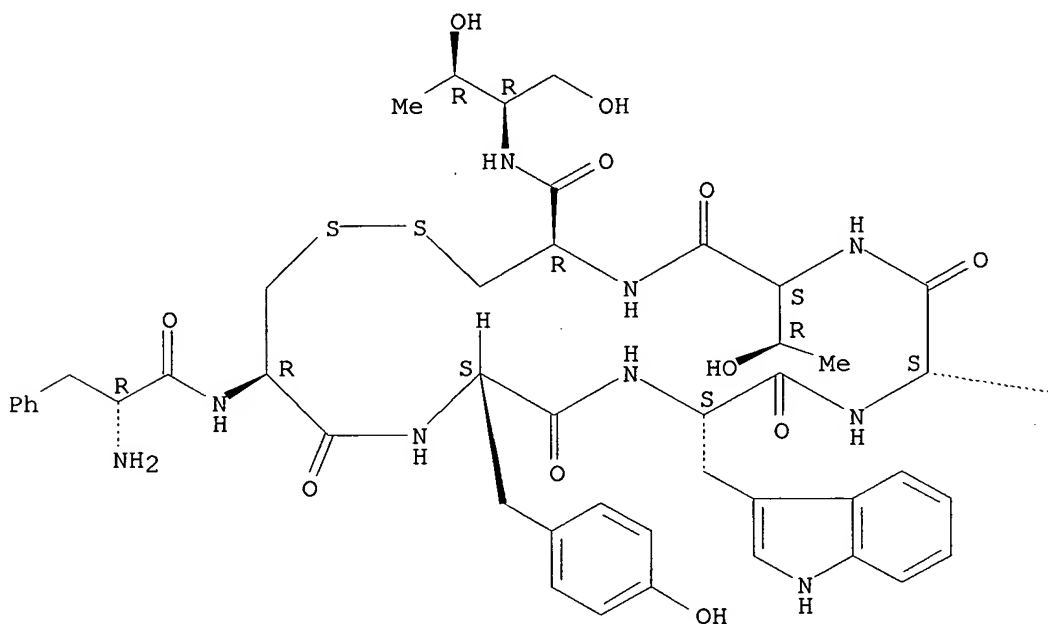
SQL 8

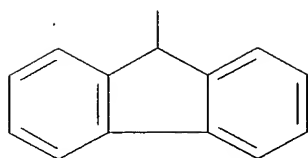
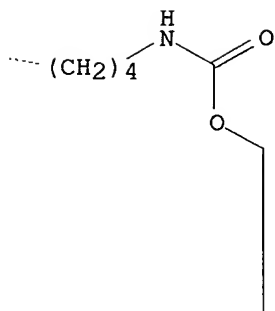
MF C64 H76 N10 O13 S2

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

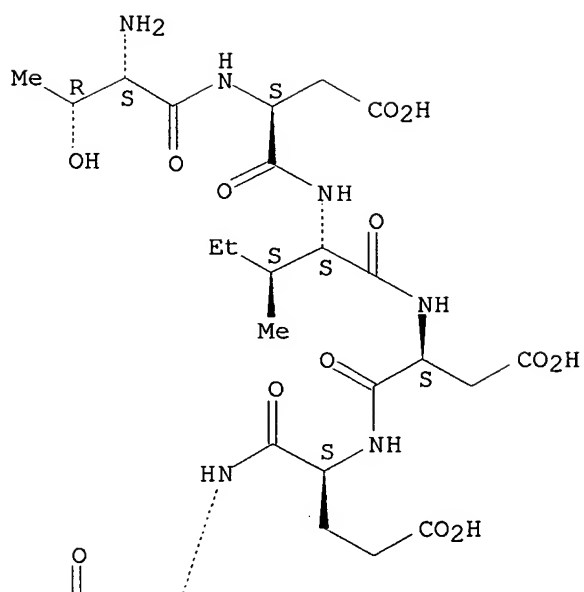
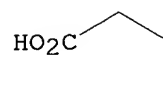
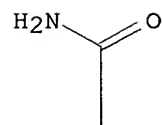




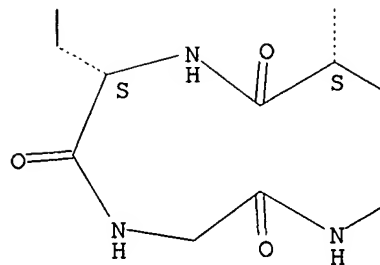
L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Glycine, L-threonyl-L-.alpha.-aspartyl-L-isoleucyl-L-.alpha.-aspartyl-L-
 .alpha.-glutamyl-L-cysteinyl-L-.alpha.-glutamyl-L-asparaginyglycylglycyl-
 L-phenylalanyl-L-cysteinyl-L-serylglycyl-L-valyl-L-cysteinyl-L-histidyl-L-
 asparaginy-L-leucyl-L-prolylglycyl-L-threonyl-L-phenylalanyl-L-.alpha.-
 glutamyl-L-cysteinyl-L-isoleucyl-L-seryl-, cyclic
 (6.fwdarw.12), (16.fwdarw.25)-bis(disulfide) (9CI)
 SQL 28
 MF C119 H174 N32 O45 S4

RELATED SEQUENCES AVAILABLE WITH SEQLINK

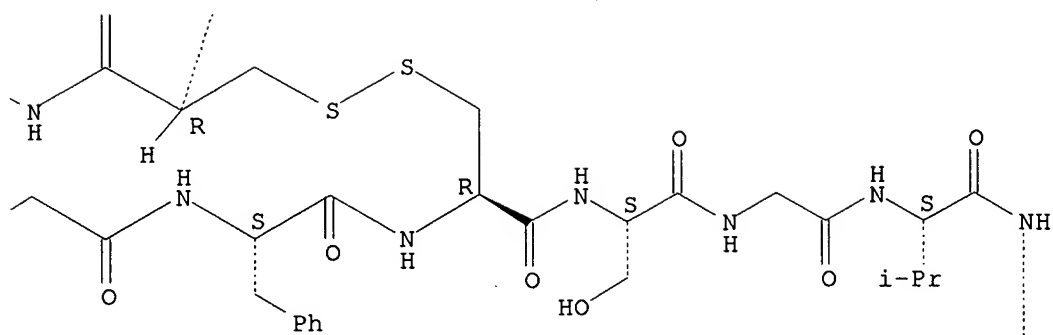
Absolute stereochemistry.



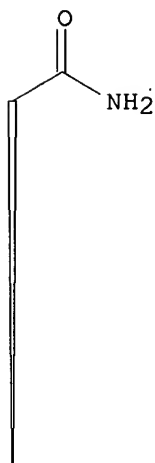
PAGE 2-A



PAGE 2-B

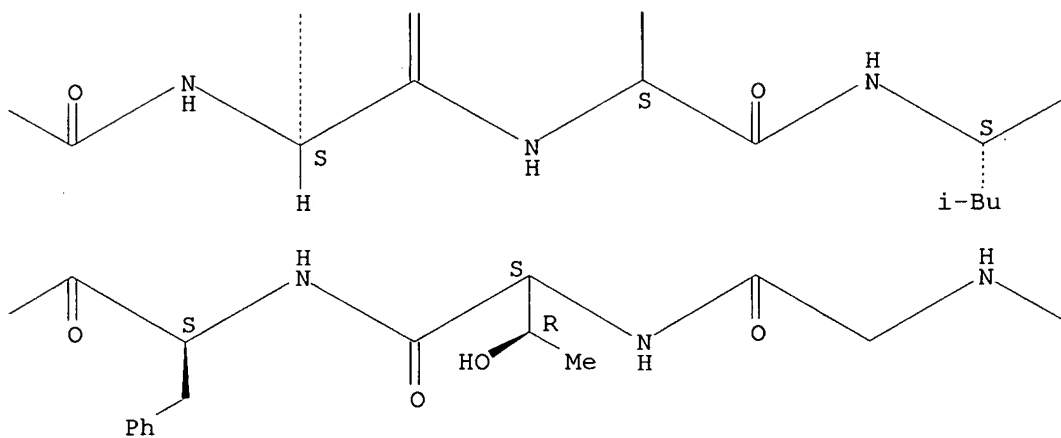
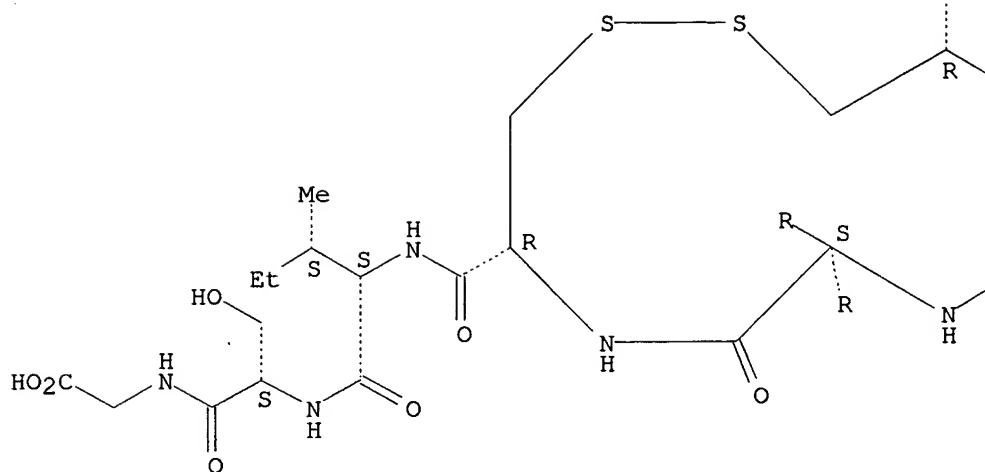


PAGE 2-C

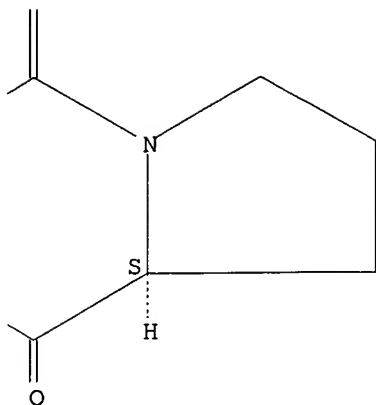


PAGE 2-D

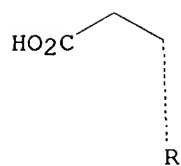




PAGE 3-D

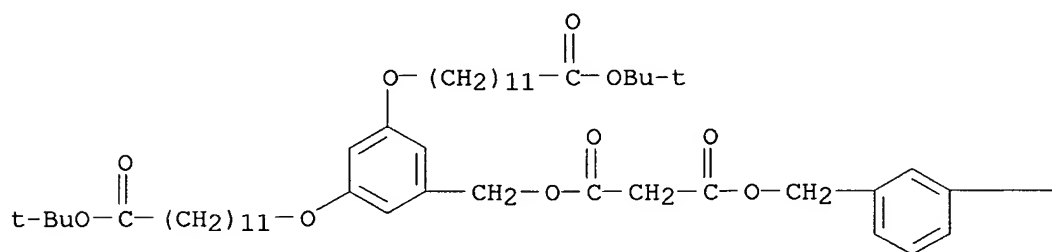


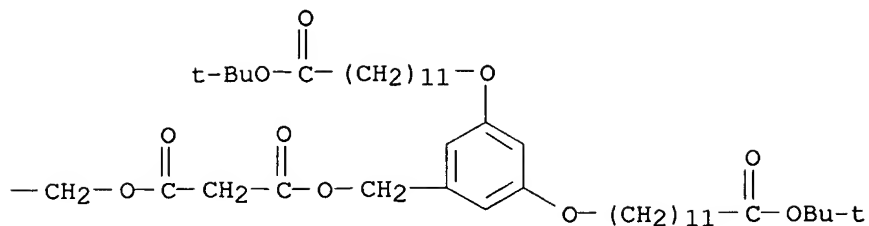
PAGE 4-A



L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Propanedioic acid, 1,3-phenylenebis(methylene) bis[[3,5-bis[[12-(1,1-dimethylethoxy)-12-oxododecyl]oxy]phenyl]methyl] ester (9CI)
 MF C92 H146 O20

PAGE 1-A

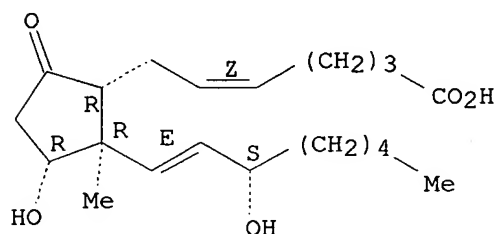




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Prosta-5,13-dien-1-oic acid, 11,15-dihydroxy-12-methyl-9-oxo-,
 (5Z,11.alpha.,13E,15S)-(.+-.)- (9CI)
 MF C21 H34 O5

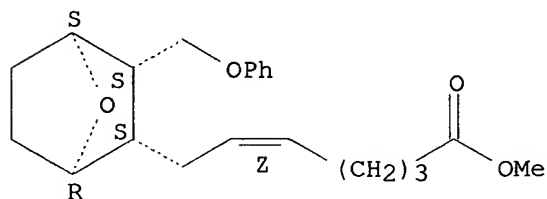
Relative stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

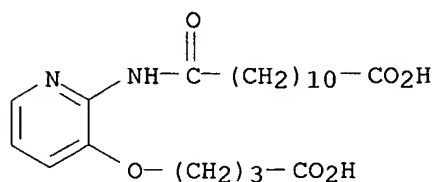
L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 5-Heptenoic acid, 7-[3-(phenoxymethyl)-7-oxabicyclo[2.2.1]hept-2-yl]-,
 methyl ester, [1R-[1.alpha.,2.alpha.(Z),3.alpha.,4.alpha.]]- (9CI)
 MF C21 H28 O4

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

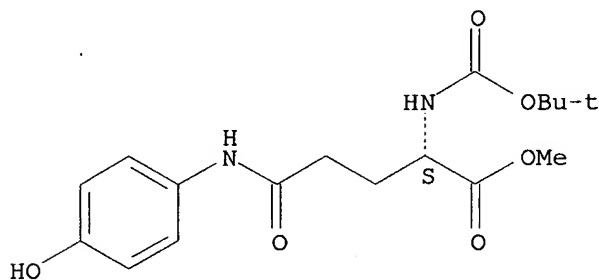
L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Dodecanoic acid, 12-[[3-(3-carboxypropoxy)-2-pyridinyl]amino]-12-oxo-
(9CI)
MF C21 H32 N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

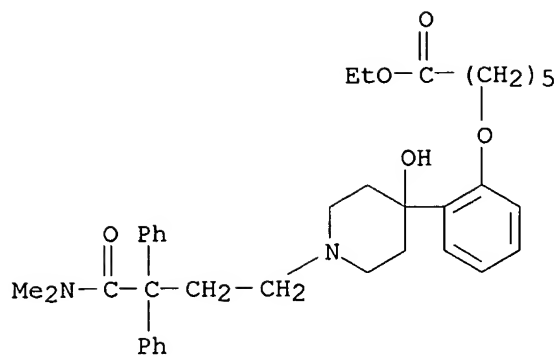
L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN L-Glutamine, N2-[(1,1-dimethylethoxy) carbonyl]-N-(4-hydroxyphenyl)-,
methyl ester (9CI)
MF C17 H24 N2 O6

Absolute stereochemistry.



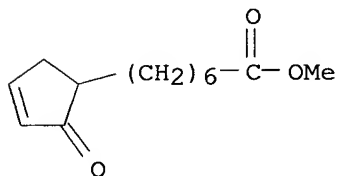
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6-[2-[1-[4-(dimethylamino)-4-oxo-3,3-diphenylbutyl]-4-
hydroxy-4-piperidinyl]phenoxy]-, ethyl ester, monohydrochloride (9CI)
MF C37 H48 N2 O5 . Cl H



● HCl

L2 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 3-Cyclopentene-1-heptanoic acid, 2-oxo-, methyl ester (9CI)
 MF C13 H20 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

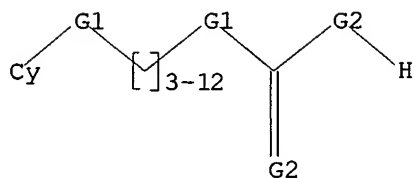
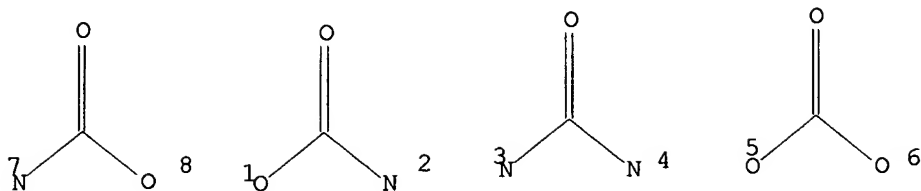
Uploading 10025947 rce first action.str

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR



G1 CH₂,O,S,N, [01-02], [03-04], [05-06], [07-08]

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search l3 sss sam

SAMPLE SEARCH INITIATED 13:43:04 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 561163 TO ITERATE

0.2% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

7 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 74805

L4 7 SEA SSS SAM L3

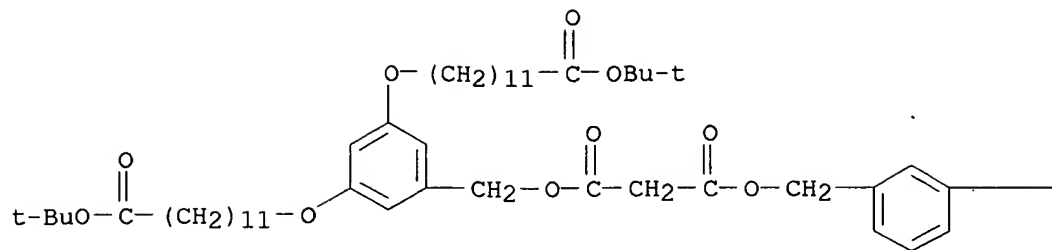
=> d scan

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS

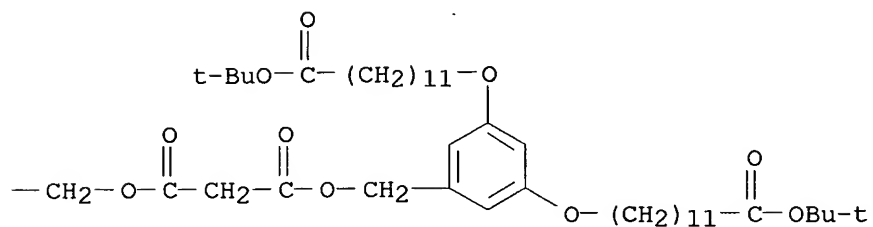
IN Propanedioic acid, 1,3-phenylenebis(methylene) bis[[3,5-bis[[12-(1,1-dimethylethoxy)-12-oxododecyl]oxy]phenyl]methyl] ester (9CI)

MF C92 H146 O20

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

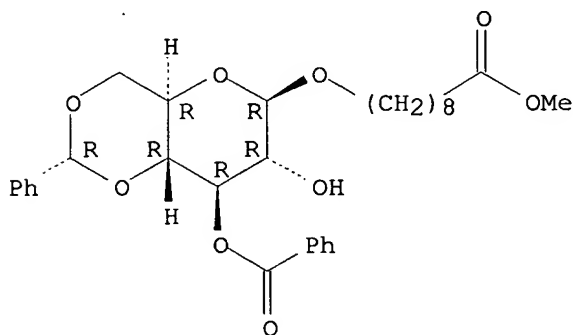
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):7

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Nonanoic acid, 9-[[3-O-benzoyl-4,6-O-(phenylmethylene)-.beta.-D-glucopyranosyl]oxy]-, methyl ester, (R)- (9CI)

MF C30 H38 O9

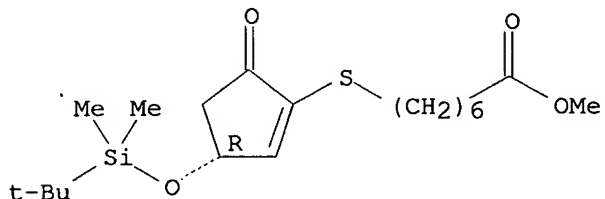
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

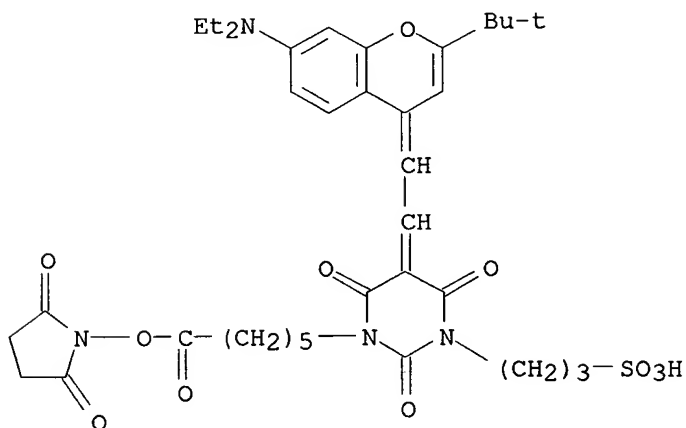
L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Heptanoic acid, 7-[[3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5-oxo-1-cyclopenten-1-yl]thio]-, methyl ester, (R)- (9CI)
 MF C19 H34 O4 S Si

Absolute stereochemistry.



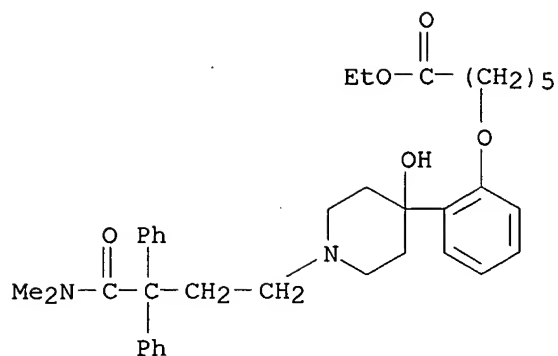
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1(2H)-Pyrimidinepropanesulfonic acid, 5-[[7-(diethylamino)-2-(1,1-dimethylethyl)-4H-1-benzopyran-4-ylidene]ethylidene]-3-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-6-oxohexyl]tetrahydro-2,4,6-trioxo-, sodium salt (9CI)
 MF C36 H46 N4 O11 S . Na



● Na

L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[2-[1-[4-(dimethylamino)-4-oxo-3,3-diphenylbutyl]-4-hydroxy-4-piperidinyl]phenoxy]-, ethyl ester, monohydrochloride (9CI)
 MF C37 H48 N2 O5 . Cl H



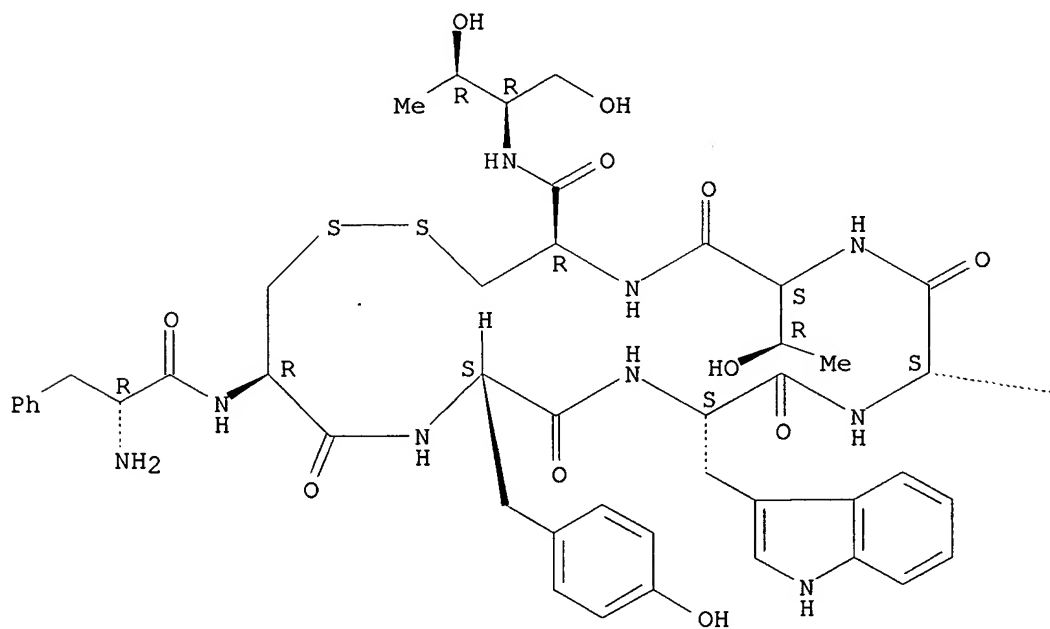
● HCl

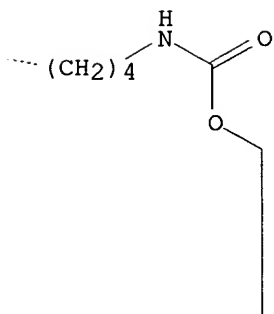
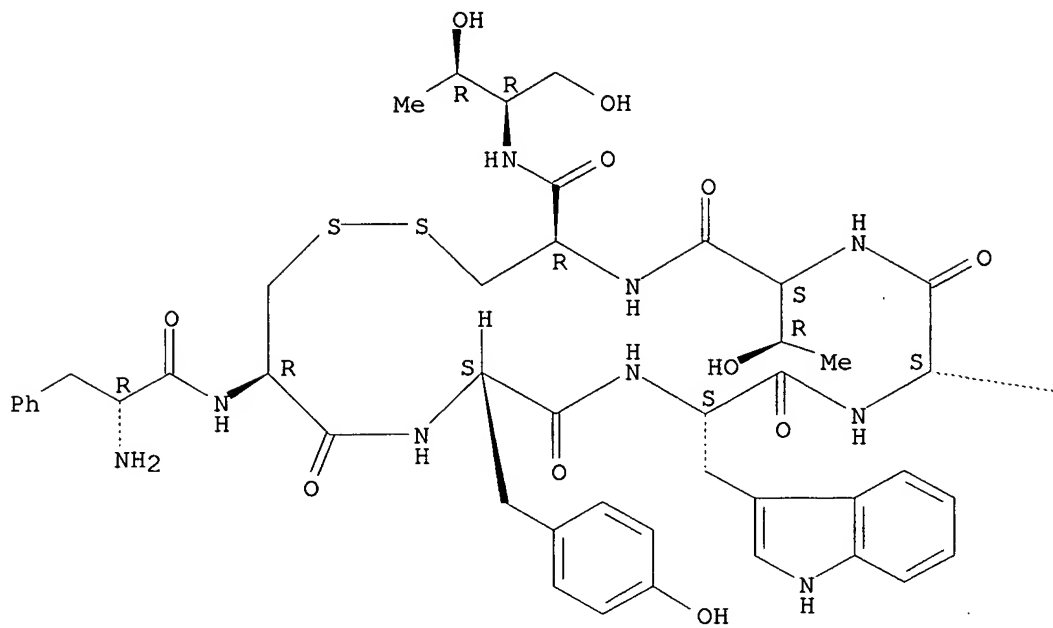
L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN L-Cysteinamide,
 D-phenylalanyl-L-cysteinyl-L-tyrosyl-L-tryptophyl-N6-[(9H-
 fluoren-9-ylmethoxy)carbonyl]-L-lysyl-L-threonyl-N-[(1R,2R)-2-hydroxy-1-
 (hydroxymethyl)propyl]-, cyclic (2.fwdarw.7)-disulfide (9CI)
 SQL 8
 MF C64 H76 N10 O13 S2

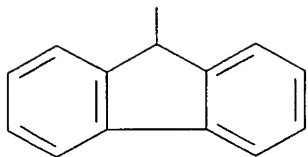
RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

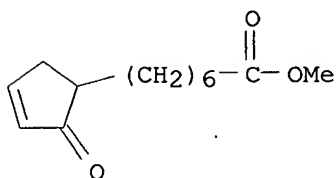
PAGE 1-A







L4 7 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 3-Cyclopentene-1-heptanoic acid, 2-oxo-, methyl ester (9CI)
 MF C13 H20 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l3 sss full
 FULL SEARCH INITIATED 13:45:17 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

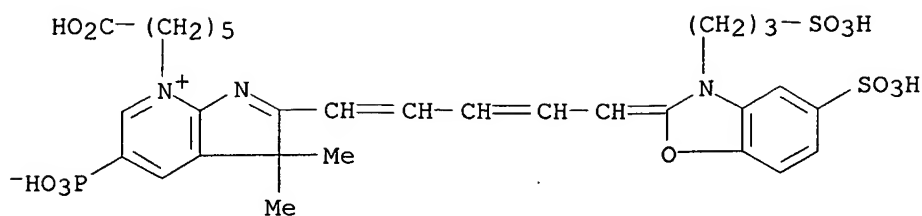
| | |
|---|--------------|
| < 3.2% PROCESSED 363804 ITERATIONS | 1424 ANSWERS |
| < 3.4% PROCESSED 382188 ITERATIONS | 1433 ANSWERS |
| < 3.6% PROCESSED 400000 ITERATIONS | 1449 ANSWERS |
| INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) | |
| SEARCH TIME: 00.02.08 | |

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
 PROJECTED ITERATIONS: EXCEEDS 1000000
 PROJECTED ANSWERS: EXCEEDS 40067

L5 1449 SEA SSS FUL L3

=> d scan

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN INDEX NAME NOT YET ASSIGNED
 MF C30 H36 N3 O12 P S2 . 2 K



● 2 K

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

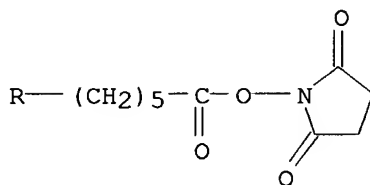
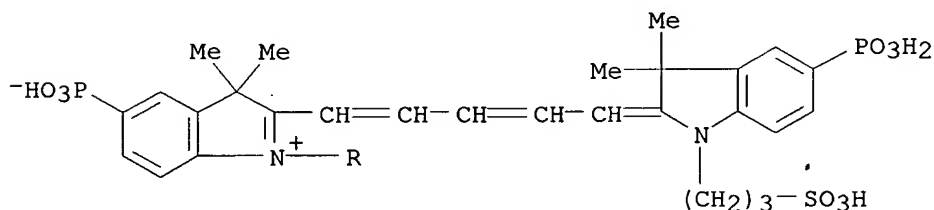
IN 3H-Indolium,

2-[5-[1,3-dihydro-3,3-dimethyl-5-phosphono-1-(3-sulfopropyl)-

2H-indol-2-ylidene]-1,3-pentadienyl]-1-[6-[(2,5-dioxo-1-pyrrolidinyl)oxy]-

6-oxohexyl]-3,3-dimethyl-5-phosphono-, inner salt, dipotassium salt (9CI)

MF C38 H47 N3 O13 P2 S . 2 K



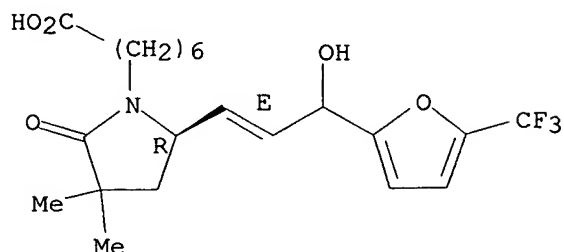
● 2 K

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1-Pyrrolidineheptanoic acid, 5-[(1E)-3-hydroxy-3-[5-(trifluoromethyl)-2-furanyl]-1-propenyl]-3,3-dimethyl-2-oxo-, (5R)- (9CI)

MF C21 H28 F3 N O5

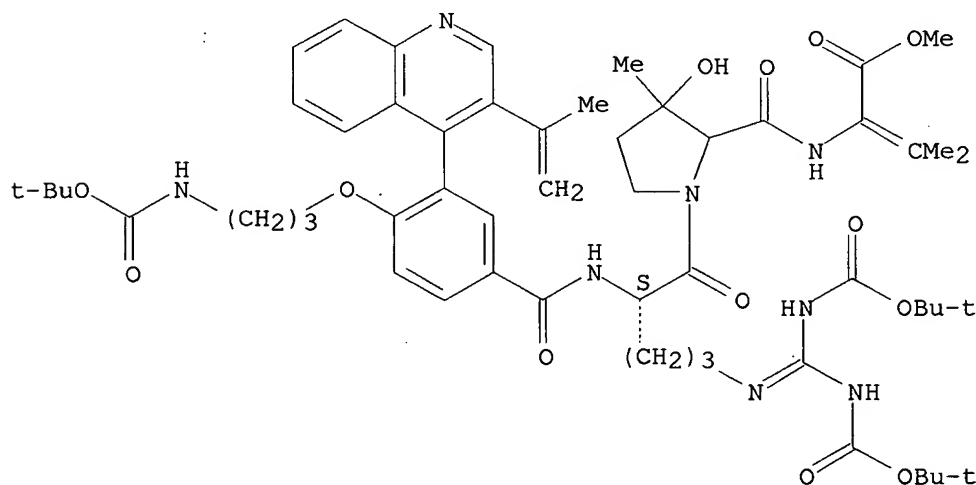
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Valine, N5-[bis[[(1,1-dimethylethoxy) carbonyl] amino]methylene]-N2-[4-[3-
[[(1,1-dimethylethoxy) carbonyl] amino]propoxy]-3-[3-(1-methylethenyl)-4-
quinolinyl]benzoyl]-L-ornithyl-3-hydroxy-3-methylpropyl-2,3-didehydro-
(9CI)
MF C55 H76 N8 O13

Absolute stereochemistry.

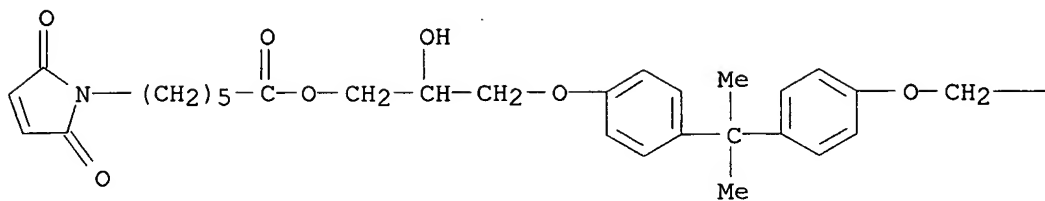


L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,2,4,5-Benzenetetracarboxylic acid, polymer with (1-
methylethylidene)bis[4,1-cyclohexanediyl]oxy(2-hydroxy-3,1-propanediyl)]
di-2-propenoate, (1-methylethylidene)bis[4,1-phenyleneoxy(2-hydroxy-3,1-
propanediyl)] bis(2,5-dihydro-2,5-dioxo-1H-pyrrole-1-hexanoate) and
.beta.,.beta.,.beta.,.beta.-tetramethyl-2,4,8,10-
tetraoxaspiro[5.5]undecane-3,9-diethanol (9CI)

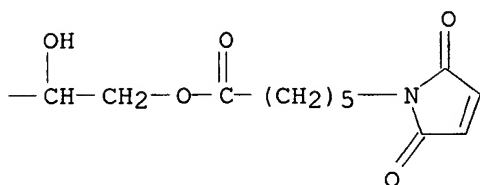
MF (C41 H50 N2 O12 . C27 H44 O8 . C15 H28 O6 . C10 H6 O8) x
 CI PMS

CM 1

PAGE 1-A

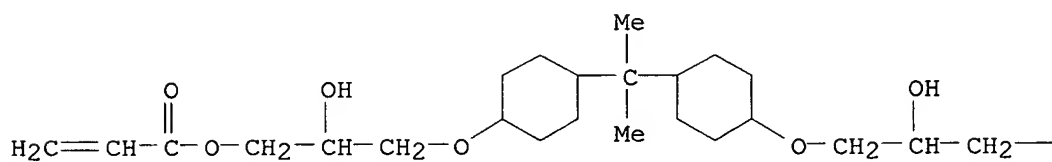


PAGE 1-B

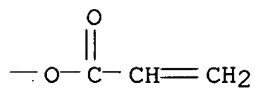


CM 2

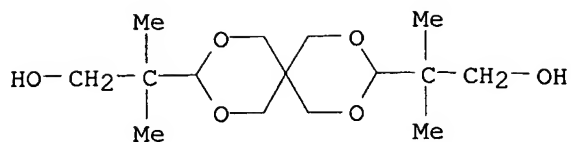
PAGE 1-A



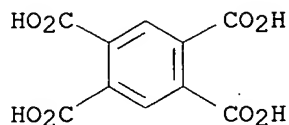
PAGE 1-B



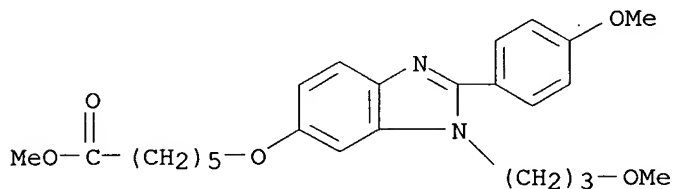
CM 3



CM 4

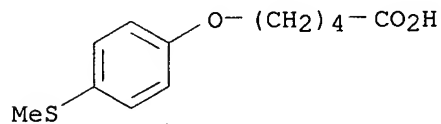


L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[[2-(4-methoxyphenyl)-1-(3-methoxypropyl)-1H-benzimidazol-
 6-yl]oxy]-, methyl ester (9CI)
 MF C25 H32 N2 O5



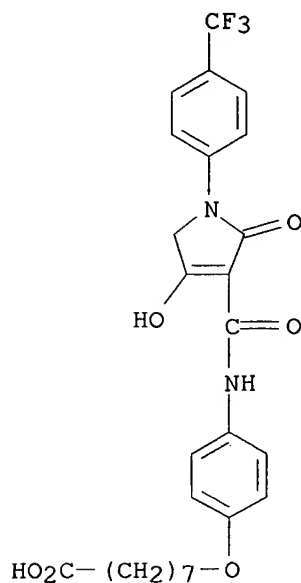
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[4-(methylthio)phenoxy]- (9CI)
 MF C12 H16 O3 S



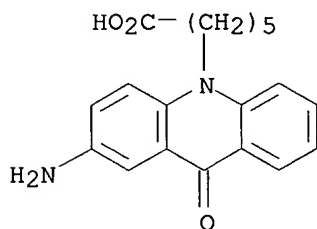
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-[4-[[[2,5-dihydro-4-hydroxy-2-oxo-1-[4-(trifluoromethyl)phenyl]-1H-pyrrol-3-yl]carbonyl]amino]phenoxy]- (9CI)
 MF C26 H27 F3 N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 10(9H)-Acridinehexanoic acid, 2-amino-9-oxo- (9CI)
 MF C19 H20 N2 O3

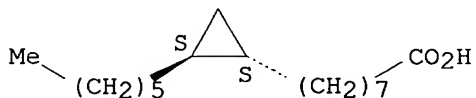


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

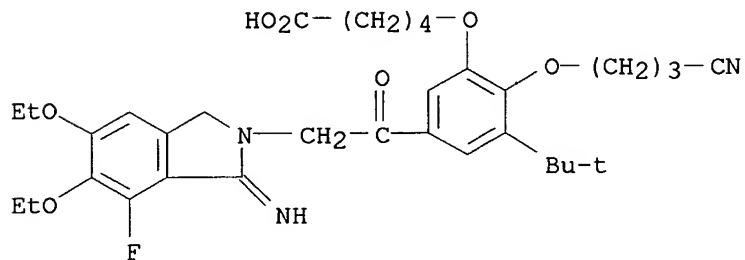
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2H-Pyran-4-carboxylic acid,
 4-[[4-(4-carboxybutoxy)phenyl]sulfonyl]tetrahy

CCCCOC(=O)C1(OCCOCC1)S(=O)(=O)c2ccc(OCCCCC(=O)O)cc2

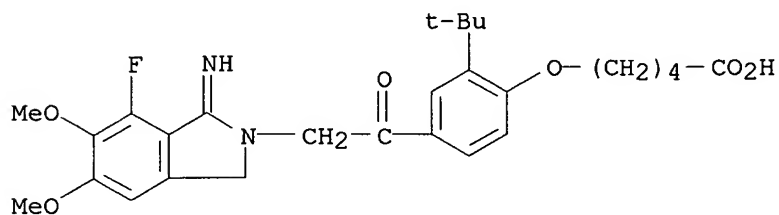
Relative stereochemistry.



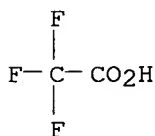
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L5 1449 ANSWERS  REGISTRY  COPYRIGHT 2003 ACS
IN  Pentanoic acid, 5-[2-(3-cyanopropoxy)-5-[(5,6-diethoxy-7-fluoro-1,3-
    dihydro-1-imino-2H-isoindol-2-yl)acetyl]-3-(1,1-dimethylethyl)phenoxy]-,
    monohydrobromide (9CI)
MF  C33 H42 F N3 O7 . Br H
```

HB γ

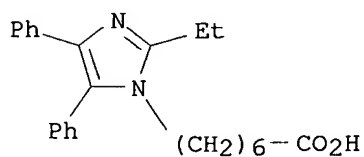
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-dihydro-1-imino-
 5,6-dimethoxy-2H-isindol-2-yl)acetyl]phenoxy]-, mono(trifluoroacetate)
 (9CI)
 MF C27 H33 F N2 O6 . C2 H F3 O2
 CM 1



CM 2



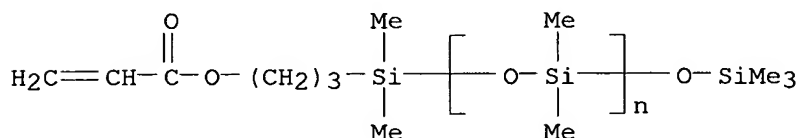
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1H-Imidazole-1-heptanoic acid, 2-ethyl-4,5-diphenyl-, monohydrochloride
 (9CI)
 MF C24 H28 N2 O2 . Cl H



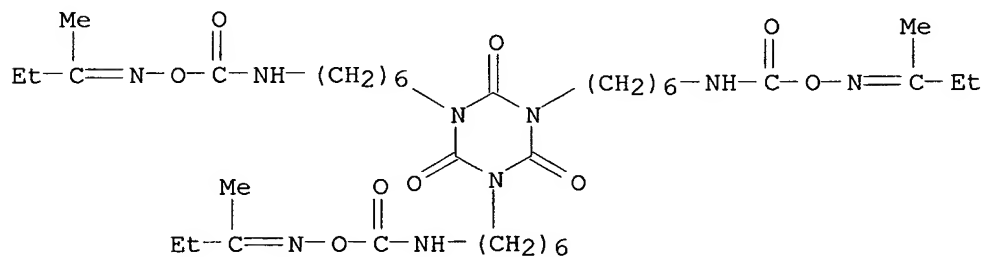
● HCl

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Neodecanoic acid, oxiranylmethyl ester, polymer with butyl
 2-methyl-2-propenoate, butyl 2-propenoate, .alpha.-[dimethyl[3-[(1-oxo-2-

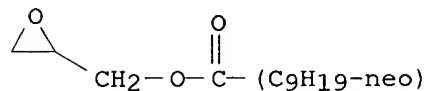
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MF      (C36 H63 N9 O9 . C13 H24 O3 . C11 H20 O2 . C8 H14 O2 . C8 H14 O2 . C8 H8
.
      C7 H12 O2 . C6 H10 O3 . C5 H8 O2 . C3 H4 O2 . (C2 H6 O Si)n C11 H24 O3
      Si2)x
CI      PMS
      CM      1      .
```



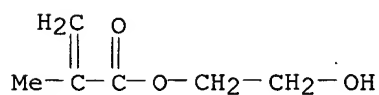
CM 2



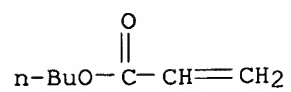
CM 3



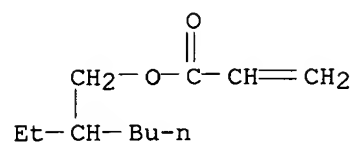
CM 4



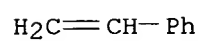
CM 5



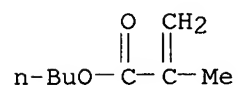
CM 6



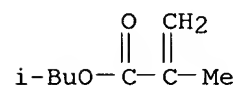
CM 7



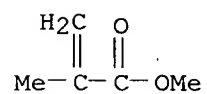
CM 8

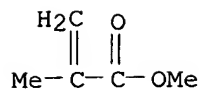


CM 9

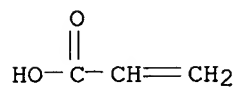


CM 10



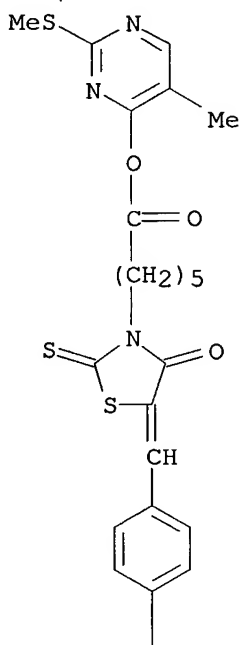


CM 11



L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 3-Thiazolidinehexanoic acid,
 5-[(4-methoxyphenyl)methylene]-4-oxo-2-thioxo-
 , 5-methyl-2-(methylthio)-4-pyrimidinyl ester (9CI)
 MF C23 H25 N3 O4 S3

PAGE 1-A

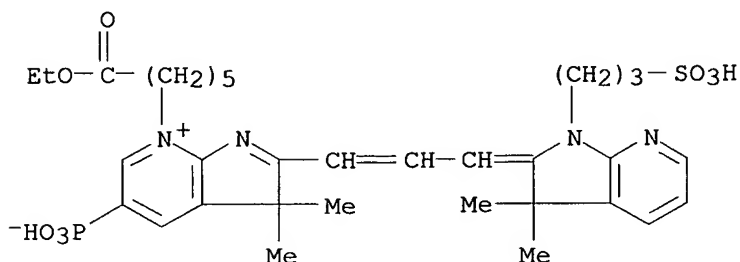


PAGE 2-A



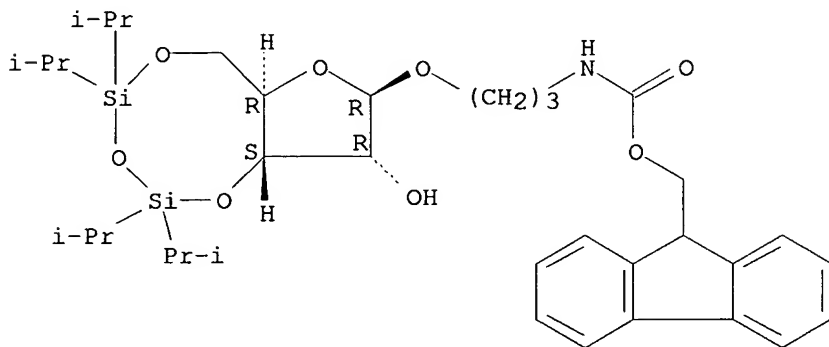
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 3H-Pyrrolo[2,3-b]pyridinium, 2-[3-[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-pyrrolo[2,3-b]pyridin-2-ylidene]-1-propenyl]-7-(6-ethoxy-6-oxohexyl)-3,3-dimethyl-5-phosphono-, inner salt (9CI)
MF C32 H43 N4 O8 P S
CI COM

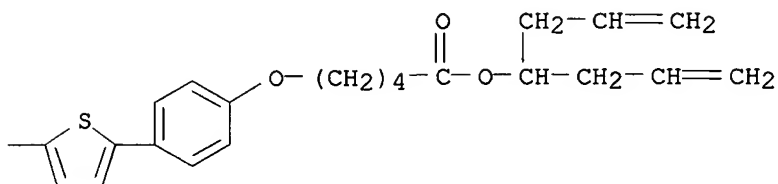
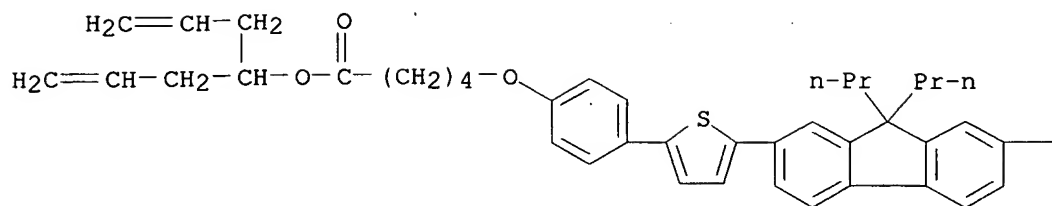


L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C35 H53 N O8 Si2

Absolute stereochemistry.



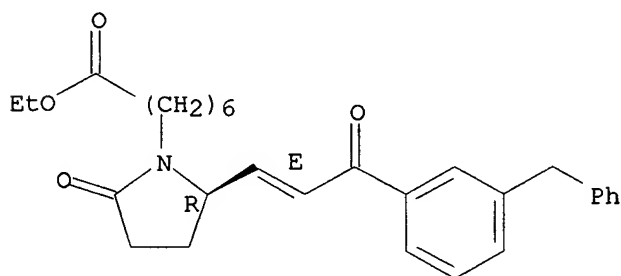
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN INDEX NAME NOT YET ASSIGNED
MF C63 H70 O6 S2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

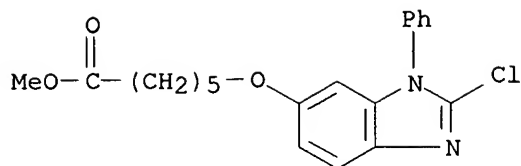
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Pyrrolidineheptanoic acid, 2-oxo-5-[(1E)-3-oxo-3-[3-(phenylmethyl)phenyl]-1-propenyl]-, ethyl ester, (5R)- (9CI)
 MF C29 H35 N O4

Absolute stereochemistry.
 Double bond geometry as shown.



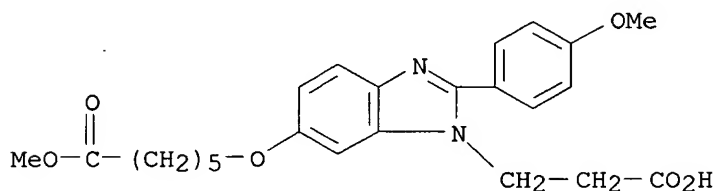
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[(2-chloro-1-phenyl-1H-benzimidazol-6-yl)oxy]-, methyl ester (9CI)
 MF C20 H21 Cl N2 O3



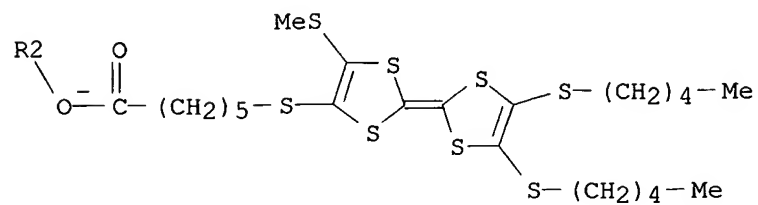
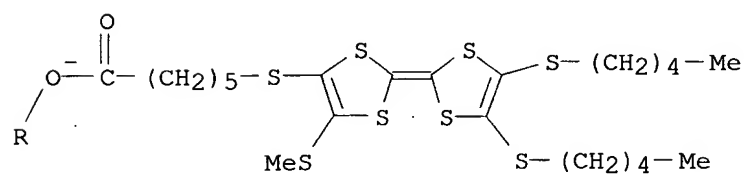
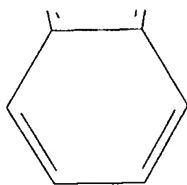
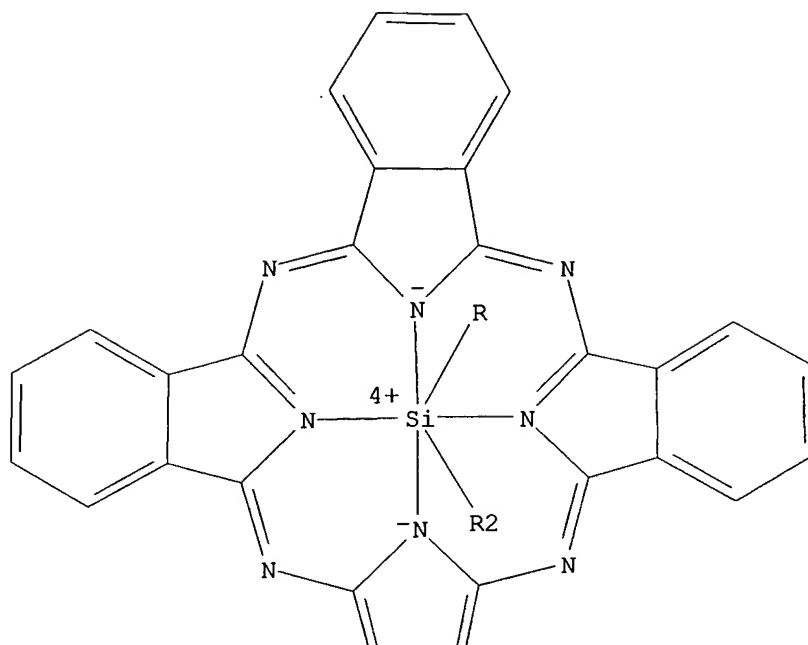
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

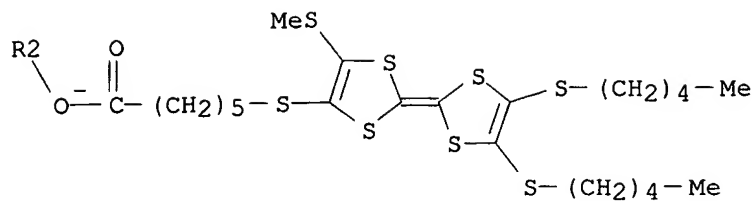
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1H-Benzimidazole-1-propanoic acid, 6-[(6-methoxy-6-oxohexyl)oxy]-2-(4-methoxyphenyl)- (9CI)
 MF C24 H28 N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Silicon, bis[6-[[2-[4,5-bis(pentylthio)-1,3-dithiol-2-ylidene]-5-(methylthio)-1,3-dithiol-4-yl]thio]hexanoato-.kappa.O][29H,31H-phthalocyaninato(2-)-.kappa.N29,.kappa.N30,.kappa.N31,.kappa.N32]-, (OC-6-12)- (9CI)
 MF C78 H86 N8 O4 S16 Si
 CI CCS

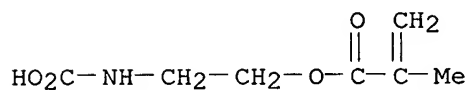




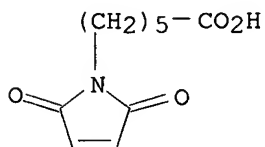
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Oxirane, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-,
 homopolymer, 6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)hexanoate
 [2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl]carbamate, homopolymer (9CI)
 MF ((C21 H24 O4)x . x C10 H13 N O4 . x C7 H11 N O4)x
 CI PMS

CM 1

CM 2

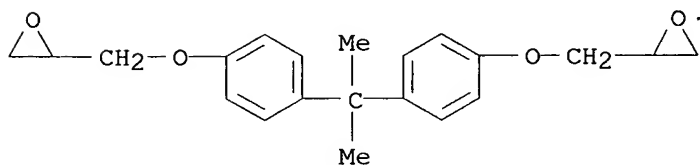


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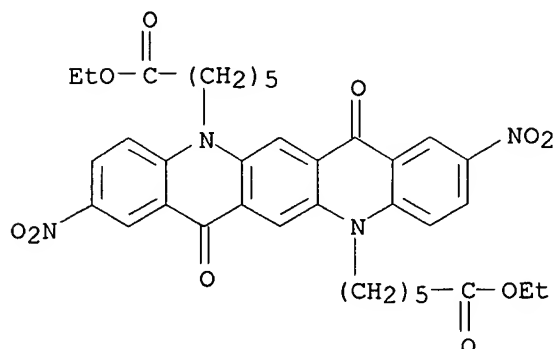


CM 4

CM 5

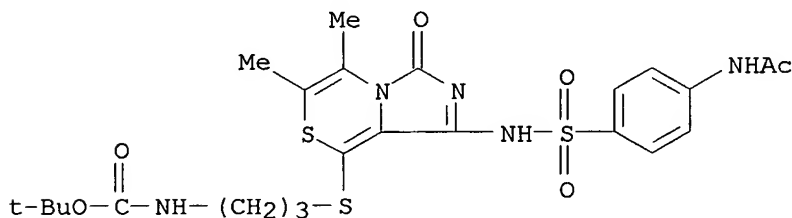


L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Quino[2,3-b]acridine-5,12-dihexanoic acid, 7,14-dihydro-2,9-dinitro-7,14-dioxo-, diethyl ester (9CI)
 MF C36 H38 N4 O10



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

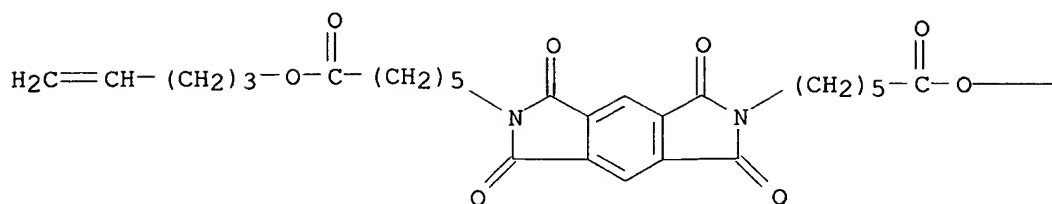
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid, [3-[[1-[[[4-(acetylamino)phenyl]sulfonyl]amino]-5,6-dimethyl-3-oxo-3H-imidazo[5,1-c][1,4]thiazin-8-yl]thio]propyl]-, 1,1-dimethylethyl ester (9CI)
 MF C24 H31 N5 O6 S3



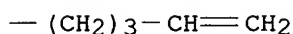
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzo[1,2-c:4,5-c']dipyrrole-2,6(1H,3H)-dihexanoic acid, 5,7-dihydro-1,3,5,7-tetraoxo-, di-4-pentenyl ester (9CI)
 MF C32 H40 N2 O8
 CI COM

PAGE 1-A

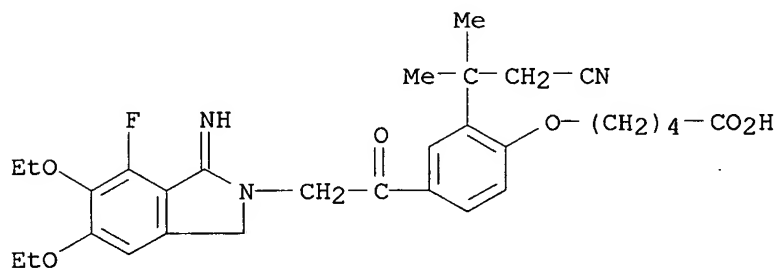


PAGE 1-B



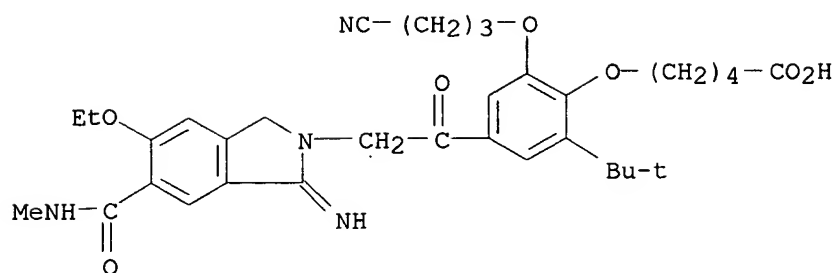
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(2-cyano-1,1-dimethylethyl)-4-[(5,6-diethoxy-7-fluoro-
 1,3-dihydro-1-imino-2H-isoindol-2-yl)acetyl]phenoxy]-, monohydrobromide
 (9CI)
 MF C30 H36 F N3 O6 . Br H



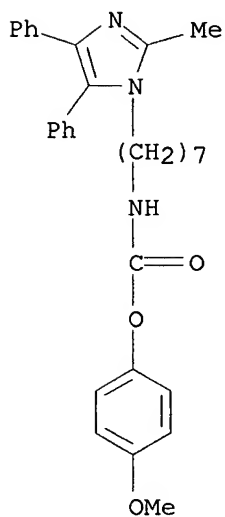
● HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[2-(3-cyanopropoxy)-6-(1,1-dimethylethyl)-4-[[5-ethoxy-
 1,3-dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2-
 yl]acetyl]phenoxy]-, monohydrobromide (9CI)
 MF C33 H42 N4 O7 . Br H



● HBr

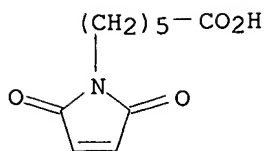
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid, [7-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)heptyl]-,
 4-methoxyphenyl ester (9CI)
 MF C31 H35 N3 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

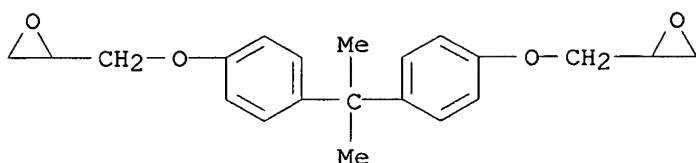
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Oxirane, 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-,
 homopolymer, 2,5-dihydro-2,5-dioxo-1H-pyrrole-1-hexanoate (9CI)
 MF (C21 H24 O4)x . x C10 H13 N O4
 CI COM

CM 1



CM 2

CM 3

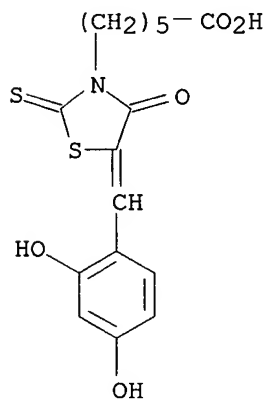


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 3-Thiazolidinehexanoic acid, 5-[(2,4-dihydroxyphenyl)methylene]-4-oxo-2-thioxo- (9CI)

MF C16 H17 N O5 S2

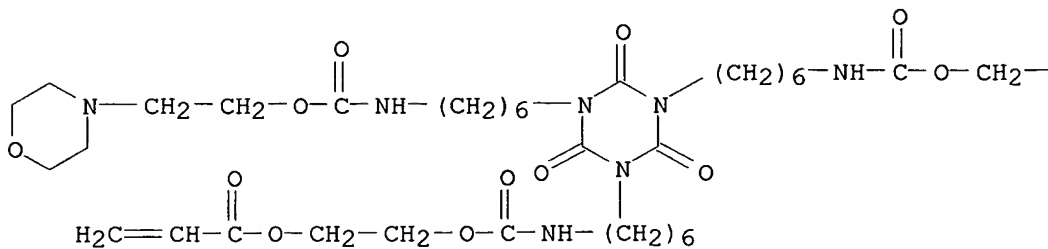


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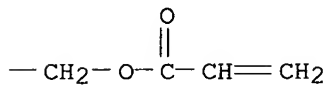
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN INDEX NAME NOT YET ASSIGNED
 MF (C40 H65 N7 O14 . C15 H24 O6 . (C2 H4 O)_n C20 H24 N2 O7)_x
 CI PMS

CM 1

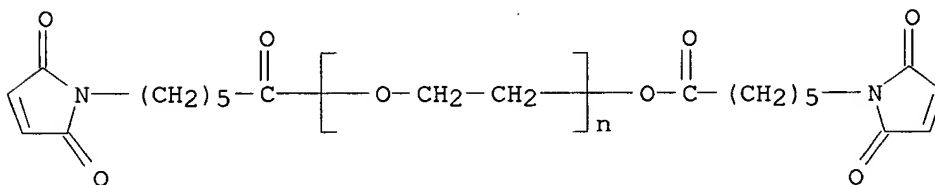
PAGE 1-A



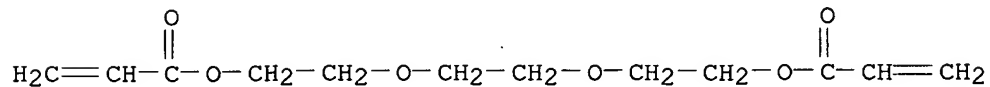
PAGE 1-B



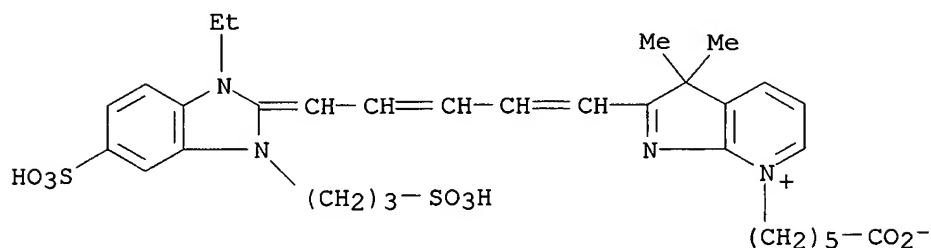
CM 2



CM 3



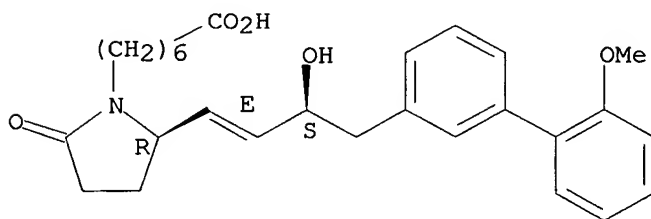
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN INDEX NAME NOT YET ASSIGNED
 MF C32 H40 N4 O8 S2 . K



● K

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Pyrrolidineheptanoic acid, 2-[(1E,3S)-3-hydroxy-4-(2'-methoxy[1,1'-biphenyl]-3-yl)-1-butenyl]-5-oxo-, (2R)- (9CI)
 MF C28 H35 N O5

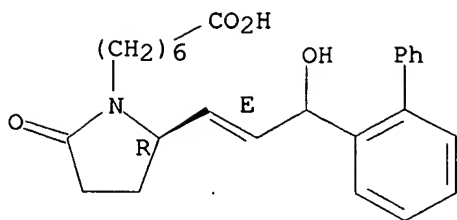
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

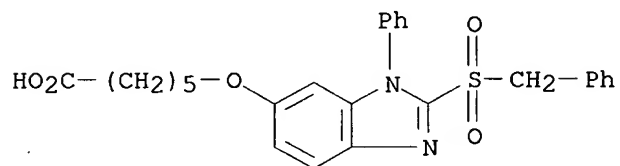
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Pyrrolidineheptanoic acid, 2-[(1E)-3-[1,1'-biphenyl]-2-yl-3-hydroxy-1-propenyl]-5-oxo-, (2R)- (9CI)
 MF C26 H31 N O4

Absolute stereochemistry.
 Double bond geometry as shown.



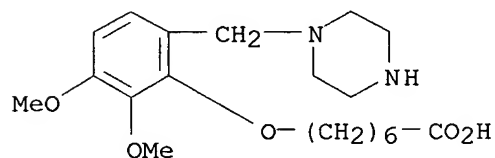
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[[1-phenyl-2-[(phenylmethyl)sulfonyl]-1H-benzimidazol-6-yl]oxy]- (9CI)
 MF C26 H26 N2 O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

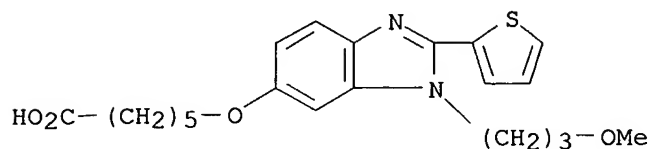
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Heptanoic acid, 7-[2,3-dimethoxy-6-(1-piperazinylmethyl)phenoxy]-, dihydrochloride (9CI)
 MF C20 H32 N2 O5 . 2 Cl H



● 2 HCl

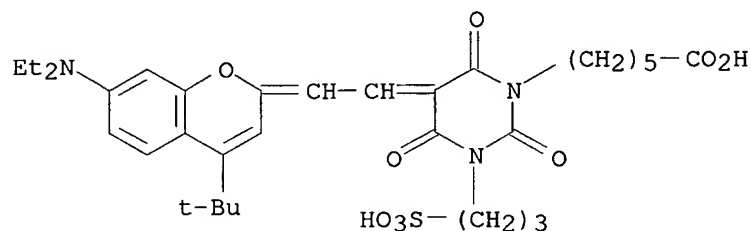
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Hexanoic acid, 6-[[1-(3-methoxypropyl)-2-(2-thienyl)-1H-benzimidazol-6-yl]oxy]- (9CI)
 MF C21 H26 N2 O4 S



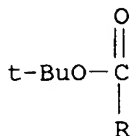
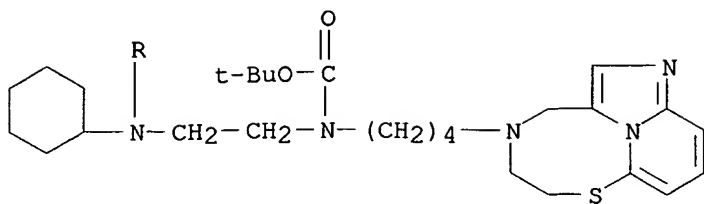
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1(2H)-Pyrimidinehexanoic acid,
 5-[[7-(diethylamino)-4-(1,1-dimethylethyl)-
 2H-1-benzopyran-2-ylidene]ethylidene]tetrahydro-2,4,6-trioxo-3-(3-
 sulfopropyl)-, monosodium salt (9CI)
 MF C32 H43 N3 O9 S . Na



● Na

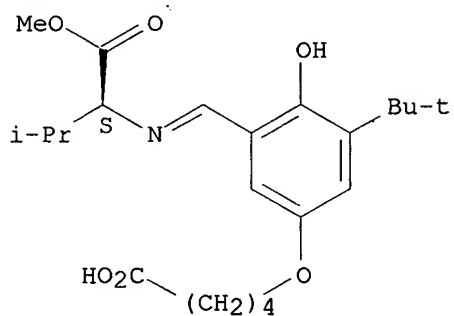
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid, cyclohexyl[2-[[4-(7,8-dihydro-6-thia-2,9,10b-
 triazacyclooct[cd]inden-9(10)-yl)butyl][(1,1-dimethylethoxy)carbonyl]amino
]ethyl]-, 1,1-dimethylethyl ester (9CI)
 MF C32 H51 N5 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[3-(1,1-dimethylethyl)-4-hydroxy-5-[[[(1S)-1-(methoxycarbonyl)-2-methylpropyl]imino]methyl]phenoxy]- (9CI)
 MF C22 H33 N O6

Absolute stereochemistry.
 Double bond geometry unknown.

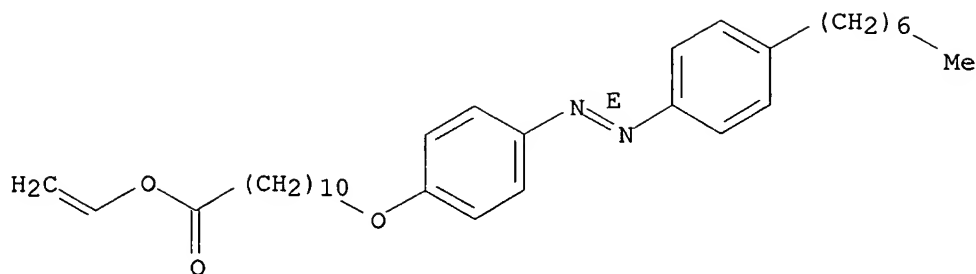


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

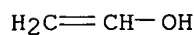
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Undecanoic acid, 11-[4-[(1E)-(4-heptylphenyl)azo]phenoxy]-, ethenyl ester,
 polymer with ethenol (9CI)
 MF (C32 H46 N2 O3 . C2 H4 O)x
 CI PMS

CM 1

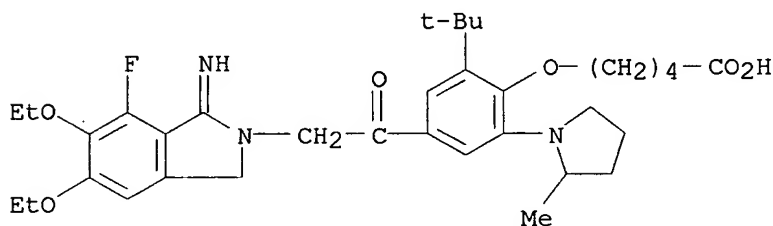
Double bond geometry as shown.



CM 2

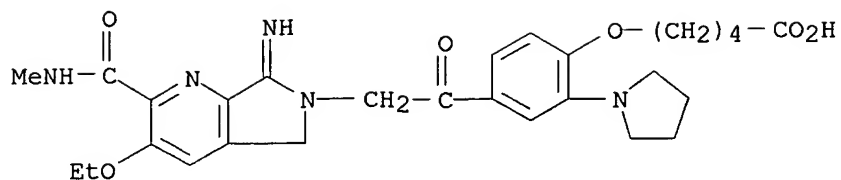


L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[4-[(5,6-diethoxy-7-fluoro-1,3-dihydro-1-imino-2H-isoindol-2-yl)acetyl]-2-(1,1-dimethylethyl)-6-(2-methyl-1-pyrrolidinyl)phenoxy]-, monohydrobromide (9CI)
 MF C34 H46 F N3 O6 . Br H



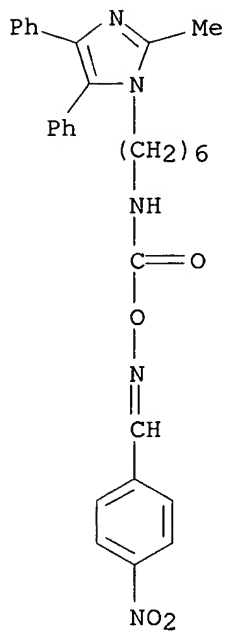
● HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[4-[[3-ethoxy-5,7-dihydro-7-imino-2-[(methylamino)carbonyl]-6H-pyrrolo[3,4-b]pyridin-6-yl]acetyl]-2-(1-pyrrolidinyl)phenoxy]-, monohydrobromide (9CI)
 MF C28 H35 N5 O6 . Br H



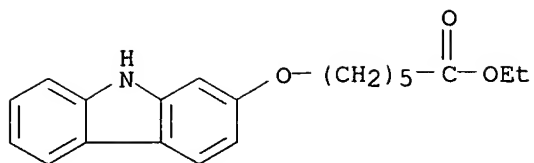
● HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzaldehyde, 4-nitro-, O-[[[6-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]amino]carbonyl]oxime (9CI)
 MF C30 H31 N5 O4



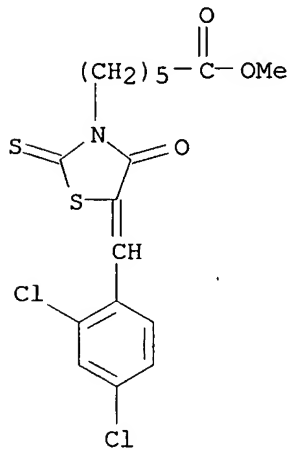
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-(9H-carbazol-2-yloxy)-, ethyl ester (9CI)
 MF C20 H23 N O3



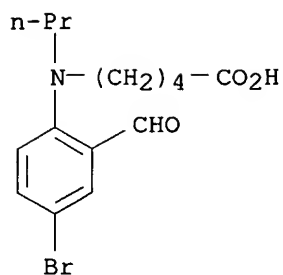
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 3-Thiazolidinehexanoic acid, 5-[(2,4-dichlorophenyl)methylene]-4-oxo-2-thioxo-, methyl ester (9CI)
 MF C17 H17 Cl2 N O3 S2



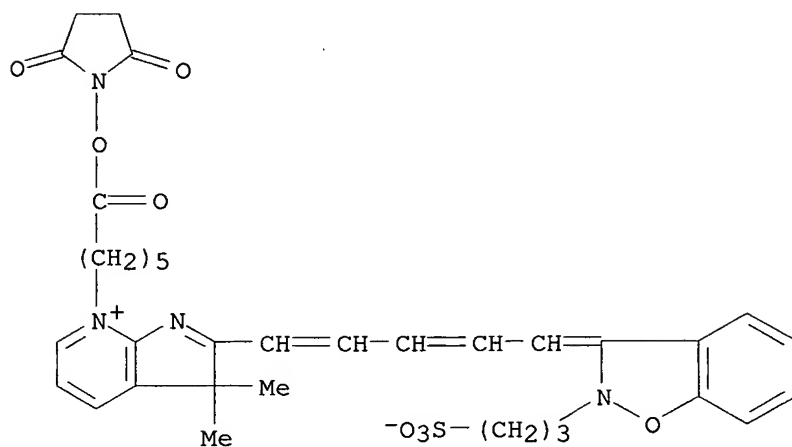
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN INDEX NAME NOT YET ASSIGNED
 MF C15 H20 Br N O3

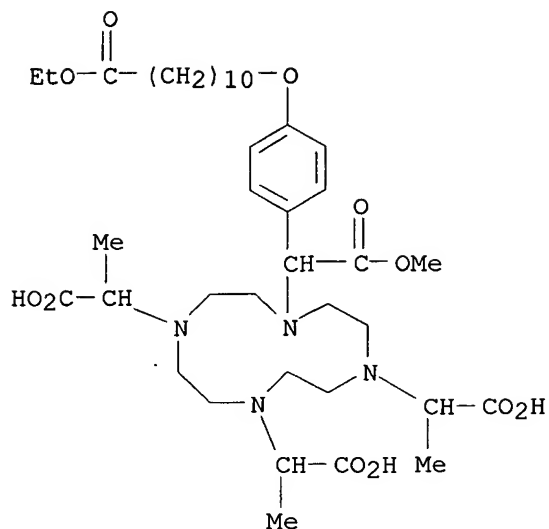


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN INDEX NAME NOT YET ASSIGNED
 MF C34 H38 N4 O8 S



L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid,
 .alpha.-[4-[(11-ethoxy-11-oxoundecyl)oxy]phenyl]-
 .alpha.',.alpha.'',.alpha.'''-trimethyl-, .alpha.-methyl ester (9CI)
 MF C39 H64 N4 O11

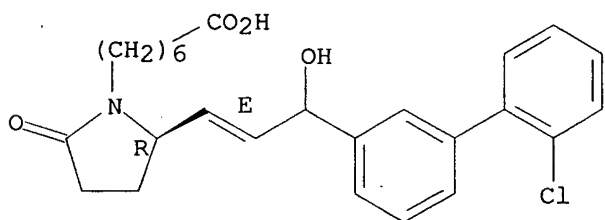


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

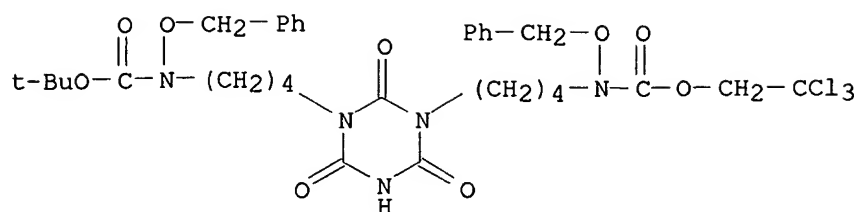
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Pyrrolidineheptanoic acid, 2-[(1E)-3-(2'-chloro[1,1'-biphenyl]-3-yl)-3-hydroxy-1-propenyl]-5-oxo-, (2R)- (9CI)
 MF C26 H30 Cl N O4

Absolute stereochemistry.
 Double bond geometry as shown.



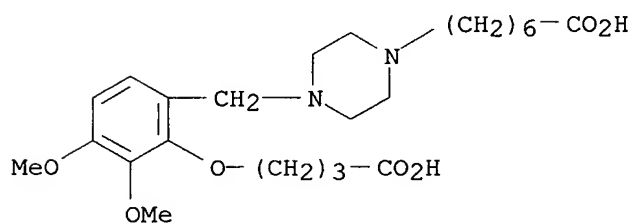
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid,
 [4-[3-[4-[[[(1,1-dimethylethoxy)carbonyl](phenylmethoxy)amino]butyl]tetrahydro-2,4,6-trioxo-1,3,5-triazin-1(2H)-yl]butyl](phenylmethoxy)-, 2,2,2-trichloroethyl ester (9CI)
 MF C33 H42 Cl3 N5 O9



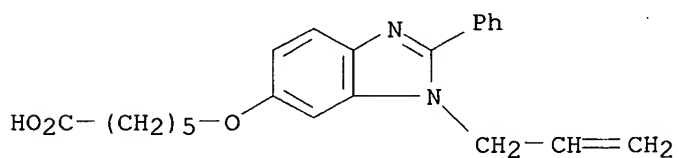
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Piperazineheptanoic acid, 4-[[2-(3-carboxypropoxy)-3,4-dimethoxyphenyl]methyl]-, dihydrochloride (9CI)
 MF C24 H38 N2 O7 . 2 Cl H



● 2 HCl

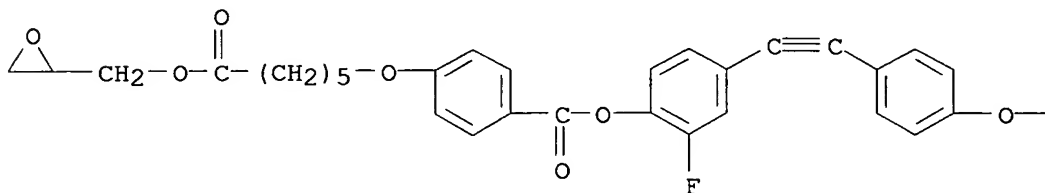
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[[2-phenyl-1-(2-propenyl)-1H-benzimidazol-6-yl]oxy]- (9CI)
 MF C22 H24 N2 O3



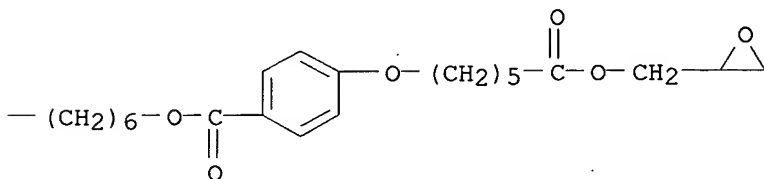
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[[6-(oxiranylmethoxy)-6-oxohexyl]oxy]-,
 2-fluoro-4-[[4-[[6-[[4-[[6-(oxiranylmethoxy)-6-
 oxohexyl]oxy]benzoyl]oxy]hexyl]oxy]phenyl]ethynyl]phenyl ester (9CI)
 MF C52 H57 F O13
 CI COM

PAGE 1-A

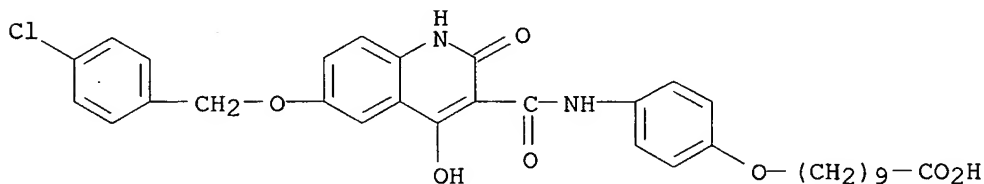


PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

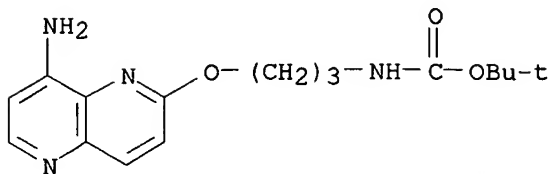
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Decanoic acid,
 10-[4-[[[6-[(4-chlorophenyl)methoxy]-1,2-dihydro-4-hydroxy-
 2-oxo-3-quinolinyl]carbonyl]amino]phenoxy]- (9CI)
 MF C33 H35 Cl N2 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid, [3-[(8-amino-1,5-naphthyridin-2-yl)oxy]propyl]-,

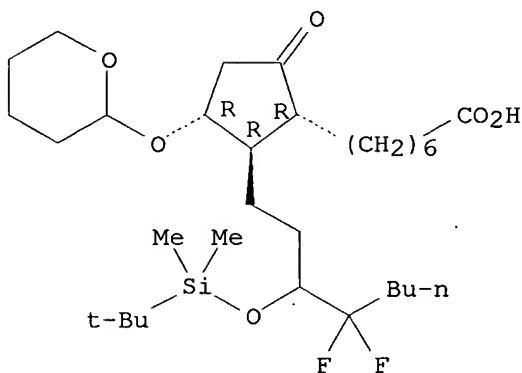
1,1-dimethylethyl ester (9CI)
 MF C16 H22 N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

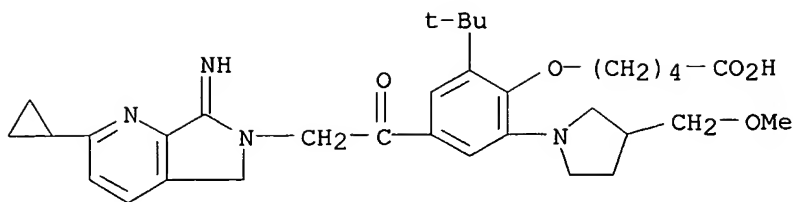
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Prostan-1-oic acid, 15-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-16,16-difluoro-9-oxo-11-[(tetrahydro-2H-pyran-2-yl)oxy]-, (11.alpha.)- (9CI)
 MF C31 H56 F2 O6 Si

Absolute stereochemistry.



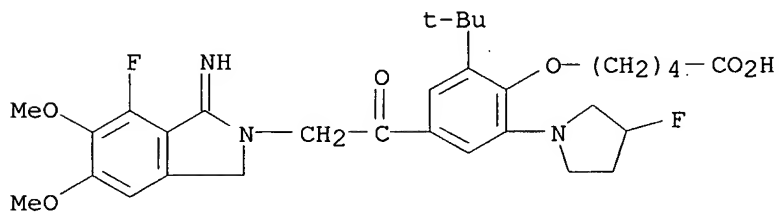
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[4-[(2-cyclopropyl-5,7-dihydro-7-imino-6H-pyrrolo[3,4-b]pyridin-6-yl)acetyl]-2-(1,1-dimethylethyl)-6-[3-(methoxymethyl)-1-pyrrolidinyl]phenoxy]-, monohydrobromide (9CI)
 MF C33 H44 N4 O5 . Br H



● HBr

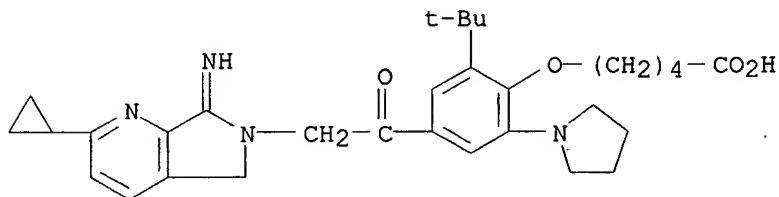
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-dihydro-1-imino-
 5,6-dimethoxy-2H-isoindol-2-yl)acetyl]-6-(3-fluoro-1-pyrrolidinyl)phenoxy]-
 , monohydrobromide (9CI)
 MF C31 H39 F2 N3 O6 . Br H



● HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[4-[(2-cyclopropyl-5,7-dihydro-7-imino-6H-pyrrolo[3,4-
 b]pyridin-6-yl)acetyl]-2-(1,1-dimethylethyl)-6-(1-pyrrolidinyl)phenoxy]-,
 mono(trifluoroacetate) (9CI)
 MF C31 H40 N4 O4 . C2 H F3 O2

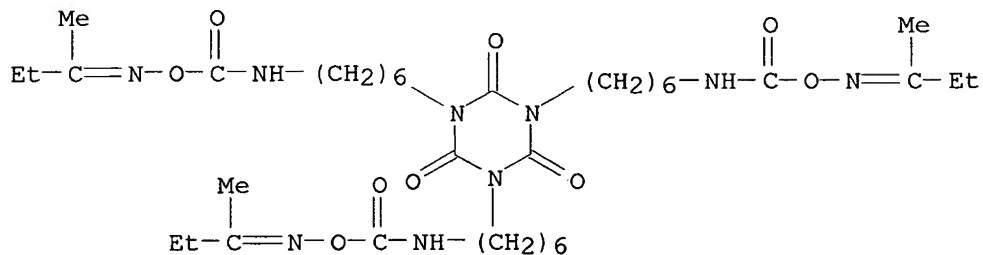
CM 1



$$\begin{array}{c} \text{F} \\ | \\ \text{F}-\text{C}-\text{CO}_2\text{H} \\ | \\ \text{F} \end{array}$$

CM 1

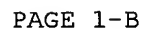
CM 2


$$\begin{array}{c} \text{OEt} \\ | \\ \text{EtO}-\text{Si}-(\text{CH}_2)_3-\text{NH}_2 \\ | \\ \text{OEt} \end{array}$$

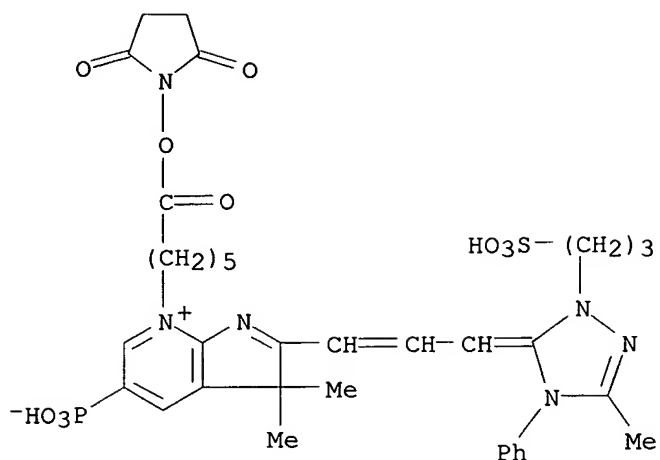
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L5 1449 ANSWERS  REGISTRY  COPYRIGHT 2003 ACS
IN 2H-Isoindole-2-hexanoic acid, 1,3-dihydro-4-nitro-1,3-dioxo-,
   4-(2-cyano-3-methoxy-3-oxo-1-propenyl)-2-methoxyphenyl ester (9CI)
MF C26 H23 N3 O9
```



PAGE 1-A

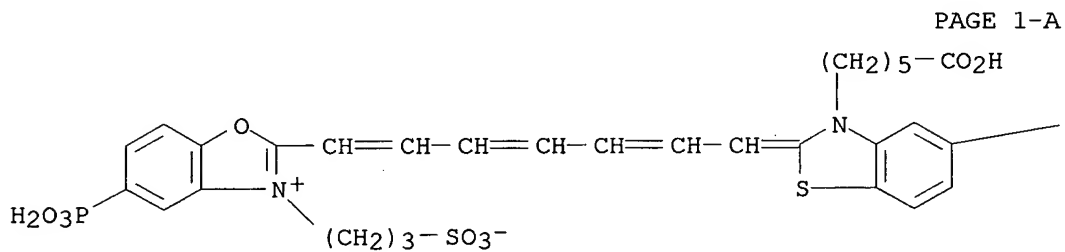


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L5 1449 ANSWERS  REGISTRY  COPYRIGHT 2003 ACS
IN 3H-Pyrrolo[2,3-b]pyridinium, 2-[3-[2,4-dihydro-5-methyl-4-phenyl-2-(3-
sulfopropyl)-3H-1,2,4-triazol-3-ylidene]-1-propenyl]-7-[6-[(2,5-dioxo-1-
pyrrolidinyl)oxy]-6-oxohexyl]-3,3-dimethyl-5-phosphono-, inner salt,
MF  C34 H41 N6 O10 P S . K
```



● K

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoxazolium, 2-[7-[3-(5-carboxypentyl)-5-phosphono-2(3H)-
 benzothiazolylidene]-1,3,5-heptatrienyl]-5-phosphono-3-(3-sulfopropyl)-,
 inner salt, dipotassium salt (9CI)
 MF C30 H34 N2 O12 P2 S2 . 2 K



● 2 K

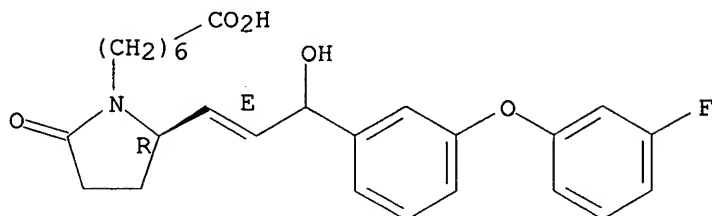
PAGE 1-B

— PO₃H₂

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1-Pyrrolidineheptanoic acid, 2-[(1E)-3-[3-(3-fluorophenoxy)phenyl]-3-hydroxy-1-propenyl]-5-oxo-, (2R)- (9CI)
 MF C26 H30 F N O5

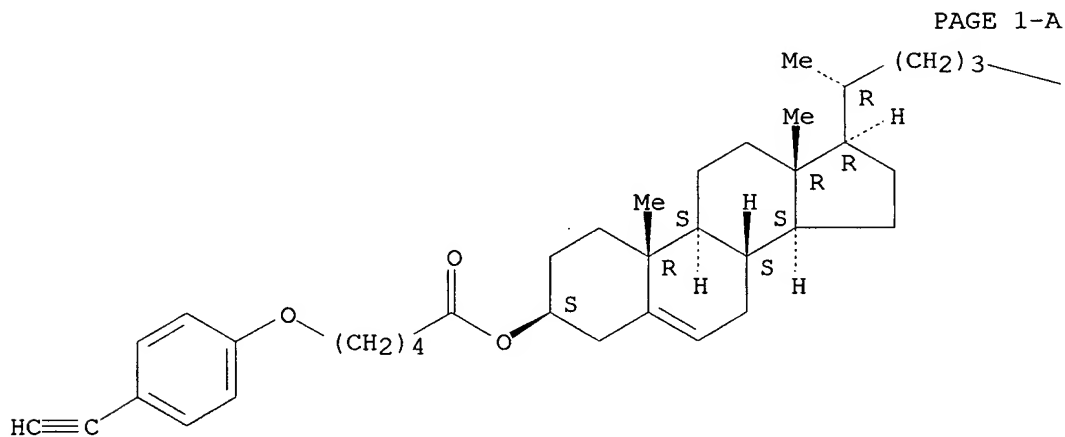
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Cholest-5-en-3-ol (3.beta.)-, 5-(4-ethynylphenoxy)pentanoate (9CI)
 MF C40 H58 O3

Absolute stereochemistry. . .

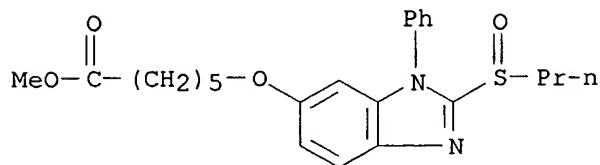


PAGE 1-B

—CHMe2

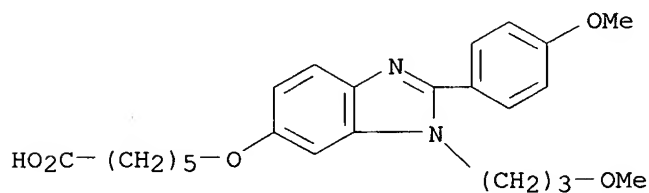
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[[1-phenyl-2-(propylsulfinyl)-1H-benzimidazol-6-yl]oxy]-,
 methyl ester (9CI)
 MF C23 H28 N2 O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

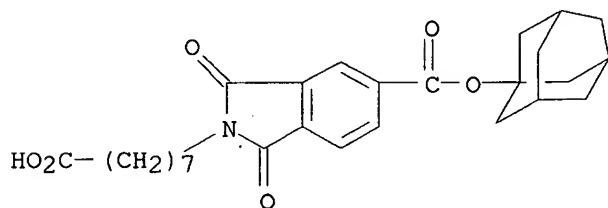
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[[2-(4-methoxyphenyl)-1-(3-methoxypropyl)-1H-benzimidazol-6-yl]oxy]- (9CI)
 MF C24 H30 N2 O5

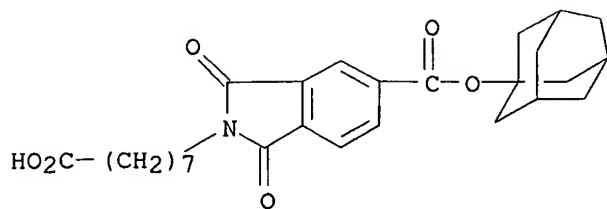


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

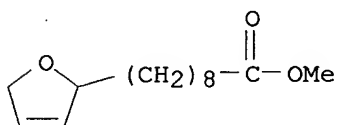
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2H-Isoindole-2-octanoic acid, 1,3-dihydro-1,3-dioxo-5-
 [(tricyclo[3.3.1.1^{3,7}]dec-1-yloxy)carbonyl]- (9CI)
 MF C27 H33 N O6





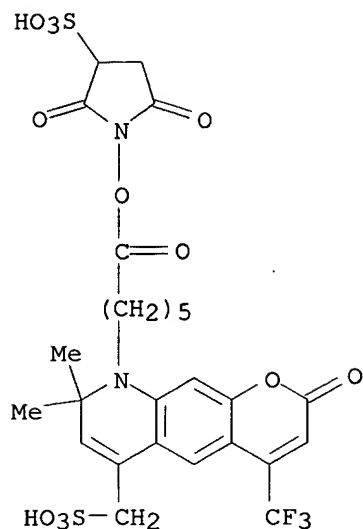
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Furannonanoic acid, 2,5-dihydro-, methyl ester (9CI)
 MF C14 H24 O3



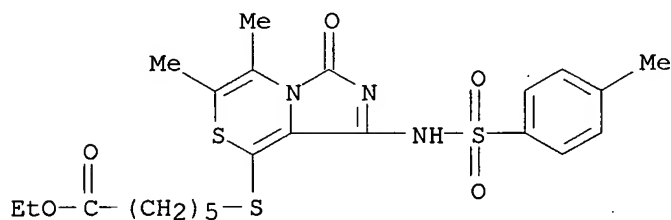
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2H-Pyrano[3,2-g]quinoline-6-methanesulfonic acid,
 9-[6-[(2,5-dioxo-3-sulfo-
 1-pyrrolidinyl)oxy]-6-oxohexyl]-8,9-dihydro-8,8-dimethyl-2-oxo-4-
 (trifluoromethyl)- (9CI)
 MF C26 H27 F3 N2 O12 S2
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

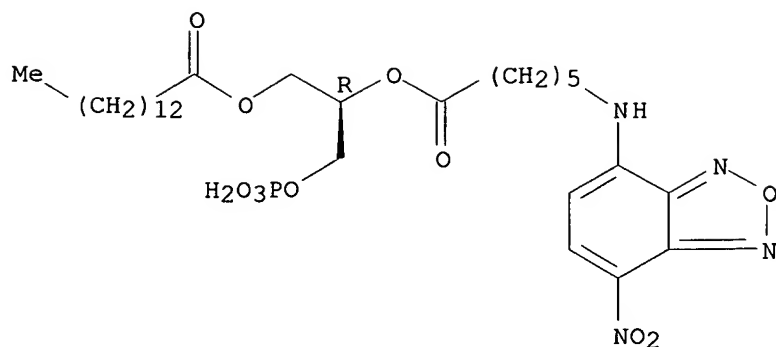
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[[5,6-dimethyl-1-[[[(4-methylphenyl)sulfonyl]amino]-3-oxo-
 3H-imidazo[5,1-c][1,4]thiazin-8-yl]thio]-, ethyl ester (9CI)
 MF C23 H29 N3 O5 S3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

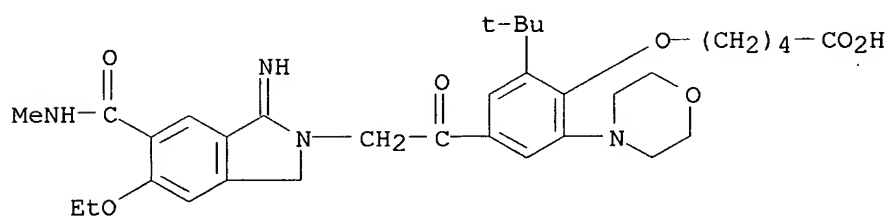
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Tetradecanoic acid,
 (2R)-2-[[[6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-1-
 oxohexyl]oxy]-3-(phosphonoxy)propyl ester, monoammonium salt (9CI)
 MF C29 H47 N4 O11 P . H3 N

Absolute stereochemistry.



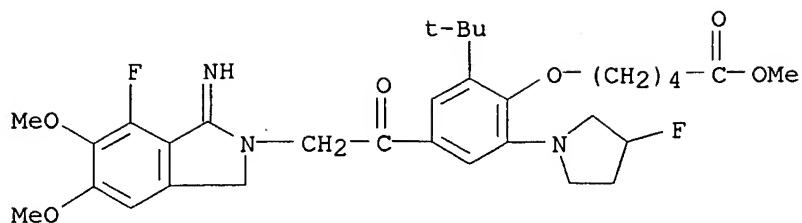
● NH₃

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-dihydro-1-imino-
 6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]-6-(4-
 morpholinyl)phenoxy]-, monohydrobromide (9CI)
 MF C33 H44 N4 O7 . Br H



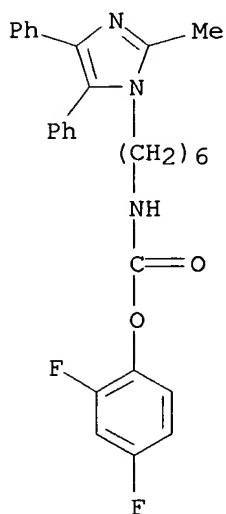
● HBr

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-dihydro-1-imino-
 5,6-dimethoxy-2H-isoindol-2-yl)acetyl]-6-(3-fluoro-1-pyrrolidinyl)phenoxy]-
 , methyl ester, monohydrochloride (9CI)
 MF C32 H41 F2 N3 O6 . Cl H



● HCl

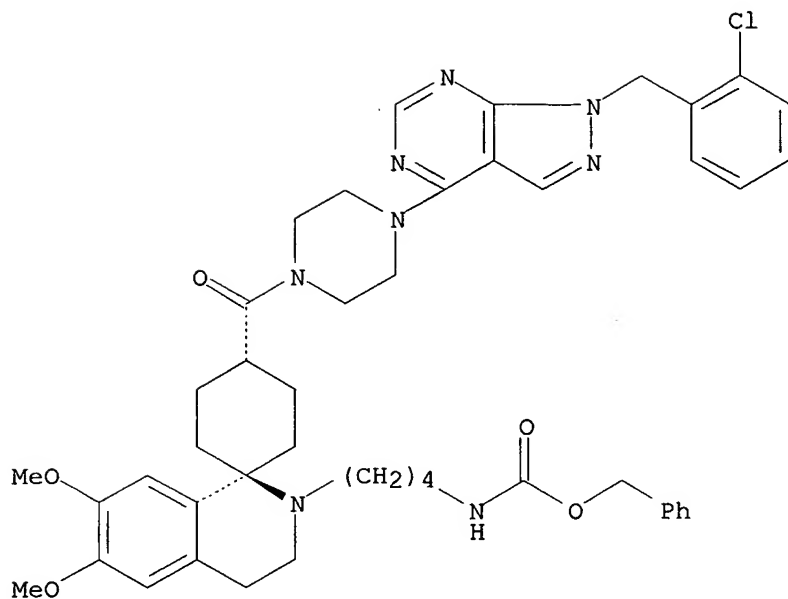
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid, [6-(2-methyl-4,5-diphenyl-1H-imidazol-1-yl)hexyl]-,
 2,4-difluorophenyl ester (9CI)
 MF C29 H29 F2 N3 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

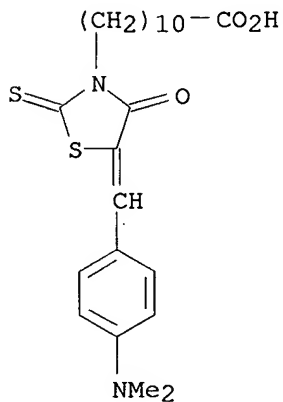
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid,
 [4-[trans-4-[[4-[1-[(2-chlorophenyl)methyl]-1H-pyrazolo[3,4-
 d]pyrimidin-4-yl]-1-piperazinyl]carbonyl]-3',4'-dihydro-6',7'-
 dimethoxyspiro[cyclohexane-1,1'(2'H)-isoquinolin]-2'-yl]butyl]-,
 phenylmethyl ester (9CI)
 MF C45 H53 Cl N8 O5

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 3-Thiazolidineundecanoic acid, 5-[[4-(dimethylamino)phenyl]methylene]-4-
 oxo-2-thioxo- (9CI)
 MF C23 H32 N2 O3 S2



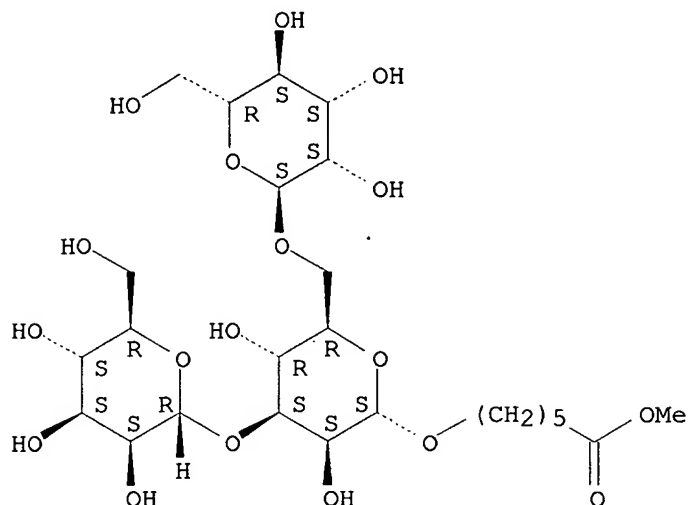
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[(O-.alpha.-D-mannopyranosyl-(1.fwdarw.3)-O-[.alpha.-D-

mannopyranosyl-(1 \rightarrow 6)]-. α -D-mannopyranosyl)oxy]-, methyl ester
(9CI)

MF C25 H44 O18

Absolute stereochemistry. Rotation (+).

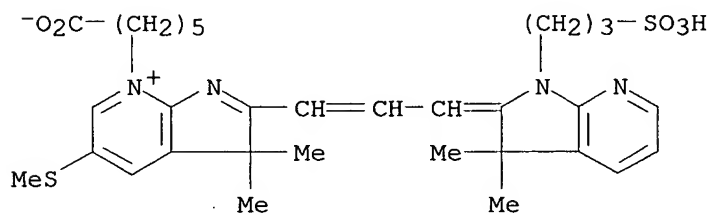


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 3H-Pyrrolo[2,3-b]pyridinium, 7-(5-carboxypentyl)-2-[3-[1,3-dihydro-3,3-dimethyl-1-(3-sulfopropyl)-2H-pyrrolo[2,3-b]pyridin-2-ylidene]-1-propenyl]-3,3-dimethyl-5-(methylthio)-, inner salt (9CI)

MF C31 H40 N4 O5 S2

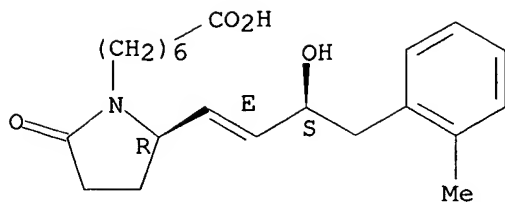


L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 1-Pyrrolidineheptanoic acid, 2-[(1E,3S)-3-hydroxy-4-(2-methylphenyl)-1-butenyl]-5-oxo-, (2R)- (9CI)

MF C22 H31 N O4

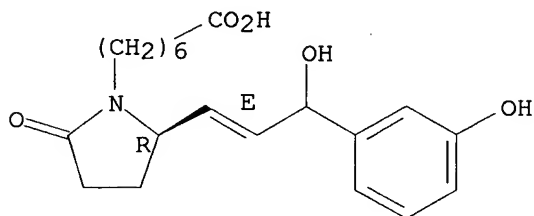
Absolute stereochemistry.
Double bond geometry as shown.



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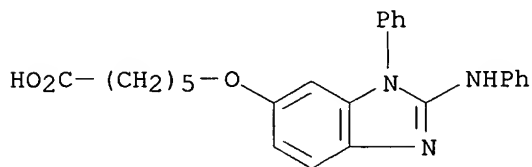
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Pyrrolidineheptanoic acid, 2-[(1E)-3-hydroxy-3-(3-hydroxyphenyl)-1-propenyl]-5-oxo-, (2R)- (9CI)
 MF C20 H27 N O5

Absolute stereochemistry.
 Double bond geometry as shown.



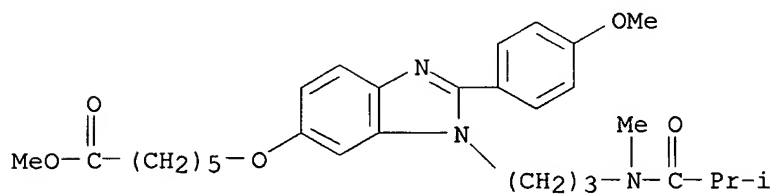
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[[1-phenyl-2-(phenylamino)-1H-benzimidazol-6-yl]oxy]- (9CI)
 MF C25 H25 N3 O3



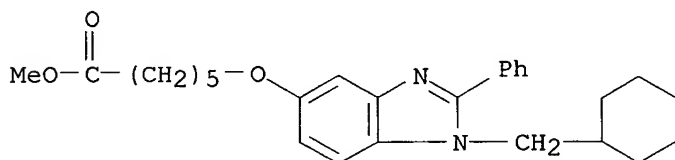
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[[2-(4-methoxyphenyl)-1-[3-[methyl(2-methyl-1-oxopropyl)amino]propyl]-1H-benzimidazol-6-yl]oxy]-, methyl ester (9CI)
 MF C29 H39 N3 O5



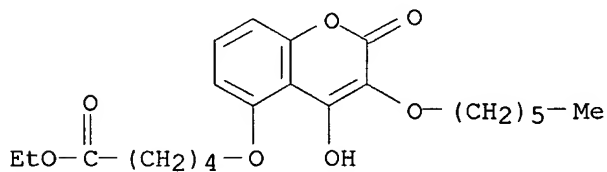
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[[1-(cyclohexylmethyl)-2-phenyl-1H-benzimidazol-5-yl]oxy]-,
 methyl ester (9CI)
 MF C27 H34 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

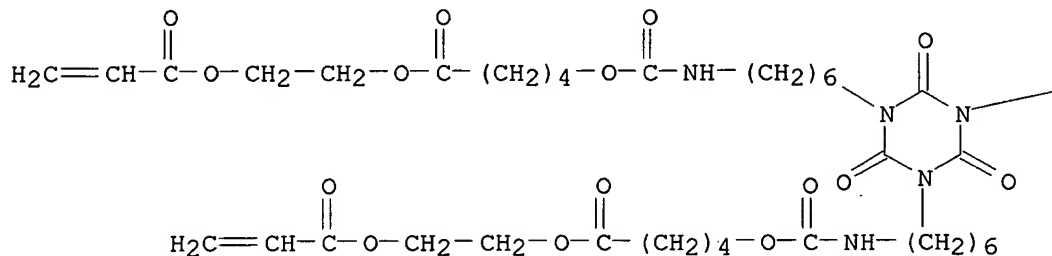
L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[[3-(hexyloxy)-4-hydroxy-2-oxo-2H-1-benzopyran-5-yl]oxy]-,
 ethyl ester (9CI)
 MF C22 H30 O7



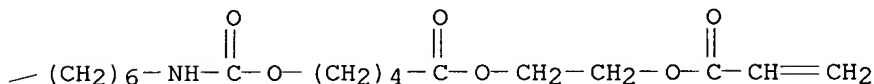
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5,5',5''-[(2,4,6-trioxo-1,3,5-triazine-1,3,5(2H,4H,6H)-
 triyl)tris(6,1-hexanediyliminocarbonyloxy)]tris-, tris[2-[(1-oxo-2-
 propenyl)oxy]ethyl] ester (9CI)
 MF C54 H84 N6 O21

PAGE 1-A

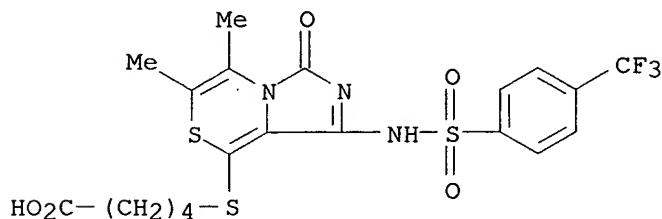


PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 1449 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[[[5,6-dimethyl-3-oxo-1-[[[4-(
 (trifluoromethyl)phenyl)sulfonyl]amino]-3H-imidazo[5,1-c][1,4]thiazin-8-
 yl]thio]- (9CI)
 MF C20 H20 F3 N3 O5 S3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp l5 gencmpds/a

ANSWER SET L5 HAS BEEN SAVED AS 'GENCMPDS/A'

=> e Hexanoic acid, 6-[[1-phenyl-2-(phenylamino)-1H-benzimidazol-6-yl]oxy]-/cn

E1 1 HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER,
S-OXI

DE, (ENDO,ANTI)-/CN
E2 1 HEXANOIC ACID, 6,7-DITHIABICYCLO(3.2.1)OCT-8-YL ESTER,
S-OXI

DE, (EXO,ANTI)-/CN
E3 0 --> HEXANOIC ACID, 6-1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-
6-YL OXY-/CN

E4 1 HEXANOIC ACID,
6-((((((3,4-DICHLOROPHENYL)METHYL)AMINO)IMIN
OMETHYL)AMINO)IMINOMETHYL)AMINO)-/CN

E5 1 HEXANOIC ACID,
6-((((((17.ALPHA.)-17-HYDROXYPREGN-4-EN-20-YN
-3-YLIDENE)AMINO)OXY)ACETYL)AMINO)-/CN

E6 1 HEXANOIC ACID,
6-((((((2-((3,5-BIS(1,1-DIMETHYLETHYL)-2-HYD

ROXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)P
HENYLACETYL)AMINO)-, (1R-(1.ALPHA.(S*),2.BETA.))-/CN

E7 1 HEXANOIC ACID,
6-((((((2-((3,5-DIBROMO-2-HYDROXYPHENYL)METH

YLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYLACETYL)AMI
NO)-, (1R-(1.ALPHA.(S*),2.BETA.))-/CN

E8 1 HEXANOIC ACID,
6-((((((2-((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-

5-METHOXYPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AM
INO)PHENYLACETYL)AMINO)-, (1R-(1.ALPHA.(S*),2.BETA.))-/CN

E9 1 HEXANOIC ACID,
6-((((((2-((3-(1,1-DIMETHYLETHYL)-2-HYDROXY-

5-NITROPHENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMIN
O)PHENYLACETYL)AMINO)-, (1R-(1.ALPHA.(S*),2.BETA.))-/CN

E10. 1 HEXANOIC ACID,
6-((((((2-((3-(1,1-DIMETHYLETHYL)-2-HYDROXYP

HENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYL
ACETYL)AMINO)-, (1R-(1.ALPHA.(S*),2.BETA.))-/CN

E11 1 HEXANOIC ACID,
6-((((((2-((5-(1,1-DIMETHYLETHYL)-2-HYDROXYP

HENYL)METHYLENE)AMINO)CYCLOHEXYL)AMINO)CARBONYL)AMINO)PHENYL
ACETYL)AMINO)-, (1R-(1.ALPHA.(S*),2.BETA.))-/CN

E12 1 HEXANOIC ACID,
6-((((((2-((2-((1-NAPHTHALENYLCARBONYL)AMINO)

-1-OXO-3-(1-(TRIPHENYLMETHYL)-1H-IMIDAZOL-4-YL)PROPYL)AMINO)
CYCLOHEXYL)OXY)CARBONYL)AMINO)ACETYL)AMINO)-,

(1S-(1.ALPHA.,

2.BETA. (R*)))-/CN

=> e Hexanoic acid, 6-((1-phenyl-2-(phenylamino)-1H-benzimidazol-6-yl)oxy)-/cn

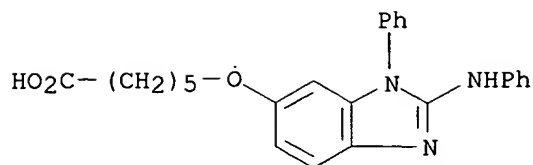
E1 1 HEXANOIC ACID,
6-((1-PHENYL-2-(4-PYRIDINYL)-1H-BENZIMIDAZOL-
6-YL)OXY)-/CN
E2 1 HEXANOIC ACID,
6-((1-PHENYL-2-(4-PYRIDINYL)-1H-BENZIMIDAZOL-
6-YL)OXY)-, METHYL ESTER/CN
E3 1 --> HEXANOIC ACID,
6-((1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-
6-YL)OXY)-/CN
E4 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-
6-YL)OXY)-, METHYL ESTER/CN
E5 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLAMINO)-1H-BENZIMIDAZOL-
6-YL)OXY)-/CN
E6 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLAMINO)-1H-BENZIMIDAZOL-
6-YL)OXY)-, METHYL ESTER/CN
E7 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLSULFINYL)-1H-BENZIMIDAZ
OL-6-YL)OXY)-, METHYL ESTER/CN
E8 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLSULFONYL)-1H-BENZIMIDAZ
OL-6-YL)OXY)-/CN
E9 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLSULFONYL)-1H-BENZIMIDAZ
OL-6-YL)OXY)-, METHYL ESTER/CN
E10 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLTHIO)-1H-BENZIMIDAZOL-6
-YL)OXY)-/CN
E11 1 HEXANOIC ACID,
6-((1-PHENYL-2-(PROPYLTHIO)-1H-BENZIMIDAZOL-6
-YL)OXY)-, METHYL ESTER/CN
E12 1 HEXANOIC ACID, 6-((1-PHENYLETHYL)AMINO)-, ETHYL ESTER/CN

=> e3

L6 1 "HEXANOIC ACID,
6-((1-PHENYL-2-(PHENYLAMINO)-1H-BENZIMIDAZOL-6-Y
L)OXY)-"/CN

=> d 16

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN 488141-30-6 REGISTRY
CN Hexanoic acid, 6-[[1-phenyl-2-(phenylamino)-1H-benzimidazol-6-yl]oxy]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C25 H25 N3 O3
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus

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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11

FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l6

L7

1 L6

=> d l7 ti fbib abs

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

TI Preparation of benzimidazoles for treatment of microglia-activation associated diseases

AN 2003:58064 CAPLUS

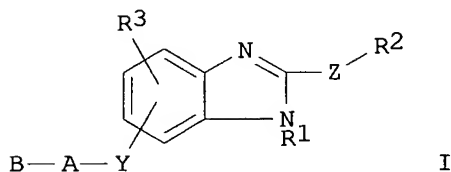
DN 138:106701

TI Preparation of benzimidazoles for treatment of microglia-activation associated diseases

IN Blume, Thorsten; Halfbrodt, Wolfgang; Kuhnke, Joachim; Moenning, Ursula; Schneider, Herbert

PA Schering Aktiengesellschaft, Germany
 SO PCT Int. Appl., 96 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|-------------------|--|----------|-------------------|----------|
| PI | WO 2003006438 | A1 | 20030123 | WO 2002-EP7561 | 20020705 |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| | DE 10135050 | A1 | 20030206 | DE 2001-10135050A | 20010709 |
| | MARPAT 138:106701 | | | DE 2001-10135050 | 20010709 |
| OS | | | | | |
| GI | | | | | |



AB The title compds. [I; R1 = (substituted) aryl, 5-6 membered heteroaryl; Z = NH, NR4, O, S, SO, SO2; R2, R4 = perfluoroalkyl, alkyl, alkylene(hetero)cyclyl, (substituted) alkylenearyl, alkyleneheteroaryl; R3 = H, F, Cl, Br, OH, OR5, OCOR5, OCONHR5, etc.; A = alkylene, alkenediyl, alkyndiyl, etc.; B = CO2H, CO2R6, CONH2, CONHNH2, etc; Y = O, NH, NR5, NCOR5, NSO2R5, etc.; R5 = CF3, C2F5, (interrupted) (substituted) alkyl, alkenyl, alkynyl, etc.; R6 = (interrupted) alkyl, alkenyl, alkynyl, etc.], were prepd. for treatment of microglia-activation assocd. diseases such as inflammatory, allergic, infectious or autoimmune diseases. Thus, 500 mg Me 6-([2-benzylmercapto-1-(4-methylphenyl)-1H-benzimidazol-6-yl]oxy)hexanoate (prepn. given) in CH2Cl2 was stirred with m-ClPhCO(OOH) for 2 h at 20.degree. to give 232 mg 6-([1-(4-methylphenyl)-2-(phenylmethylsulfonyl)-1H-benzimidazol-6-yl]oxy)hexanoic acid. The latter inhibited the microglia-activation with IC50 = 0.46 .mu.M.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

| | | |
|--|------------|---------|
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| FULL ESTIMATED COST | 3.25 | 168.71 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
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STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7
 DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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Experimental and calculated property data are now available. See HELP
 PROPERTIES for more information. See STNnote 27, Searching Properties
 in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

```
=> e Pentanoic acid, 5-(4-(methylthio)phenoxy)-/cn
E1          1      PENTANOIC ACID,
5-(4-(IMINO(( (PHENYLMETHOXY) CARBONYL) AMINO) M
              ETHYL) PHENOXY)-/CN
E2          1      PENTANOIC ACID,
5-(4-(IMINO(( (PHENYLMETHOXY) CARBONYL) AMINO) M
              ETHYL) PHENOXY)-, ETHYL ESTER/CN
E3          1 --> PENTANOIC ACID, 5-(4-(METHYLTHIO) PHENOXY)-/CN
E4          1      PENTANOIC ACID,
5-(4-ACETYL-2-ETHYL-5-HYDROXYPHENOXY)-2,2-DI
              METHYL-/CN
E5          1      PENTANOIC ACID, 5-(4-ACETYL-2-METHOXYPHENOXY)-, METHYL
ESTER
              /CN
E6          1      PENTANOIC ACID, 5-(4-ACETYL-3-HYDROXY-2-PROPYLPHENOXY)-/CN
E7          1      PENTANOIC ACID, 5-(4-ACETYL-3-HYDROXY-2-PROPYLPHENOXY)-,
ETH
              YL ESTER/CN
E8          1      PENTANOIC ACID, 5-(4-ACETYL-3-HYDROXY-2-PROPYLPHENOXY)-,
MET
              HYL ESTER/CN
E9          1      PENTANOIC ACID,
5-(4-ACETYL-5-HYDROXY-2-(2-PROPENYL) PHENOXY)
              -/CN
E10         1      PENTANOIC ACID, 5-(4-ACETYL-5-HYDROXY-2-PROPYLPHENOXY)-/CN
E11         1      PENTANOIC ACID, 5-(4-ACETYLPHENOXY)-/CN
```

E12 1 PENTANOIC ACID, 5-(4-ACETYLPHENOXY)-, METHYL ESTER/CN

=> e3

L8 1 "PENTANOIC ACID, 5-(4-(METHYLTHIO)PHENOXY)-"/CN

=> d 18

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 485795-28-6 REGISTRY

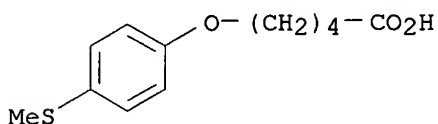
CN Pentanoic acid, 5-[4-(methylthio)phenoxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H16 O3 S

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus

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| | | |
|--|------------------|---------------|
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -0.65 |

FILE 'CAPLUS' ENTERED AT 13:57:02 ON 11 MAR 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11

FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l8

L9 1 L8

=> d l9 ti fbib abs

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

TI Polyhydroxyalkanoate with (methylsulfanyl) phenoxy structure in side chain

AN 2003:40201 CAPLUS

DN 138:105715

TI Polyhydroxyalkanoate with (methylsulfanyl) phenoxy structure in side chain

IN Kenmoku, Takashi; Sugawa, Etsuko; Yano, Tetsuya; Imamura, Takeshi

PA Canon Kabushiki Kaisha, Japan

SO Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

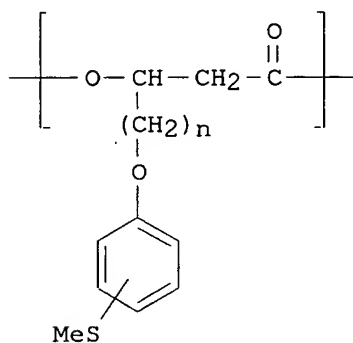
DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|------------------|----------|
| PI | EP 1275727 | A2 | 20030115 | EP 2002-15356 | 20020710 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| | | | | JP 2001-208705 A | 20010710 |

GI



I

AB A polyhydroxyalkanoate that comprises a unit represented by the chem. formula (I): wherein n is an integer of 1-8 being the same or different in the polyhydroxyalkanoate. The microbial prodn. process is also disclosed.

=>

=>

=>

Uploading 10025947 rce first action 2nd.str

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

5.75

180.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.65

-1.30

FILE 'REGISTRY' ENTERED AT 14:01:36 ON 11 MAR 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

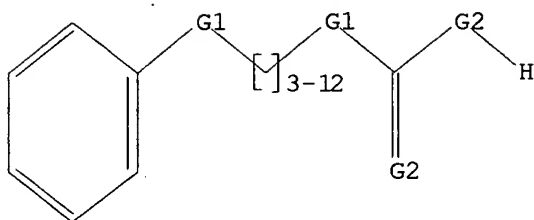
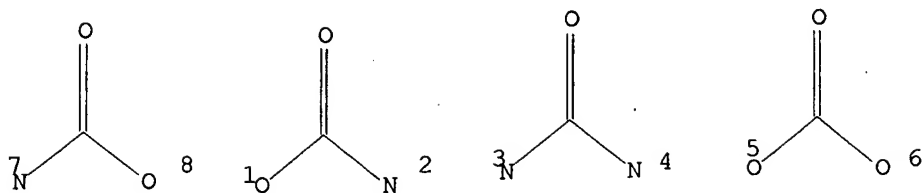
Uploading 10025947 rce first action 2nd.str

L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10 STR



G1 CH2,O,S,N, [C1-C2],[C3-C4],[C5-C6],[C7-C8]
G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search l10 sss sam

SAMPLE SEARCH INITIATED 14:02:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L11 0 SEA SSS SAM L10

=>

=>

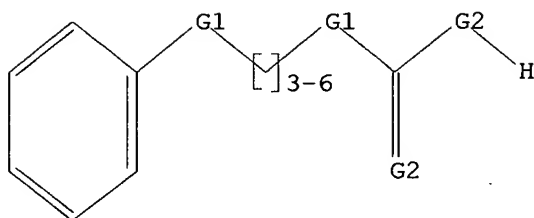
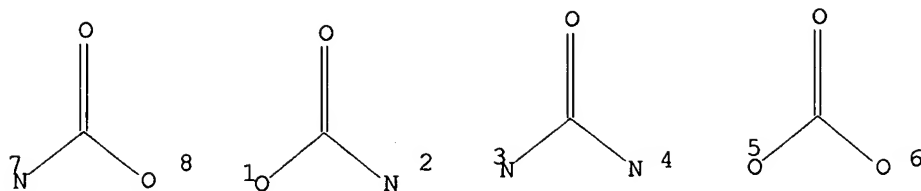
Uploading 10025947 rce first action 2nd.str

L12 STRUCTURE UPLOADED

=> d l12

L12 HAS NO ANSWERS

L12 STR



G1 CH₂,O,S,N, [C1-C2], [C3-C4], [C5-C6], [C7-C8]

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> search l12 sss sam

SAMPLE SEARCH INITIATED 14:04:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 0

L13 0 SEA SSS SAM L12

=> search l12 sss full

FULL SEARCH INITIATED 14:05:44 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 5.3% PROCESSED 400000 ITERATIONS

8 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.22

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

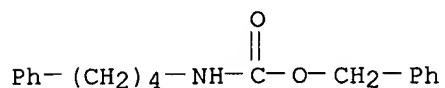
PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 115

L14 8 SEA SSS FUL L12

=> d scan

L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Carbamic acid, (4-phenylbutyl)-, phenylmethyl ester (9CI)
MF C18 H21 N O2

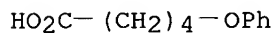


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

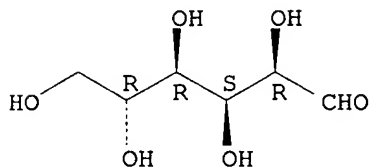
L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN D-Glucose, polymer with 5-phenoxy pentanoic acid (9CI)
MF (C11 H14 O3 . C6 H12 O6)x
CI PMS

CM 1



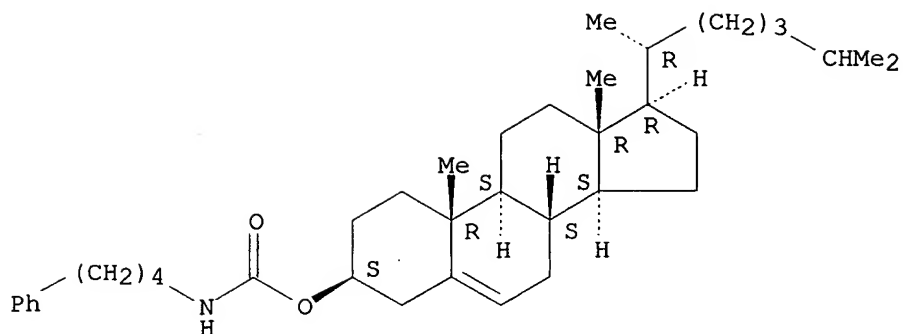
CM 2

Absolute stereochemistry.



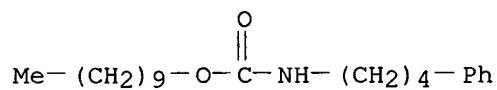
L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Cholest-5-en-3-ol (3.beta.)-, (4-phenylbutyl)carbamate (9CI)
MF C38 H59 N O2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

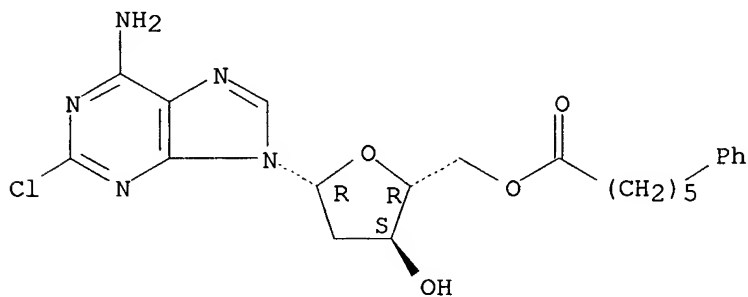
L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid, (4-phenylbutyl)-, decyl ester (9CI)
 MF C21 H35 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

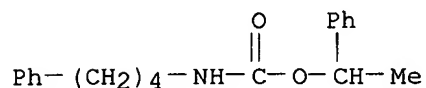
L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Adenosine, 2-chloro-2'-deoxy-, 5'-benzenehexanoate (9CI)
 MF C22 H26 Cl N5 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

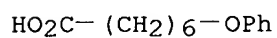
L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Carbamic acid, (4-phenylbutyl)-, 1-phenylethyl ester (9CI)
 MF C19 H23 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

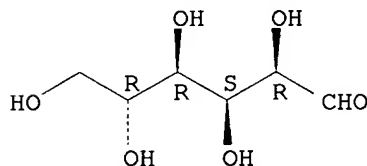
L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN D-Glucose, polymer with 7-phenoxyheptanoic acid (9CI)
 MF (C13 H18 O3 . C6 H12 O6)x
 CI PMS

CM 1



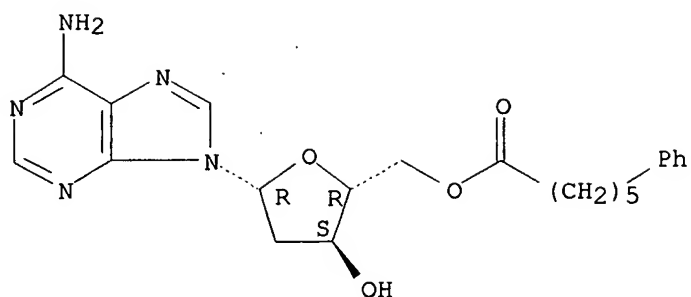
CM 2

Absolute stereochemistry.



L14 8 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Adenosine, 2'-deoxy-, 5'-benzenehexanoate (9CI)
 MF C22 H27 N5 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d cost

COST IN U.S. DOLLARS

CONNECT CHARGES

NETWORK CHARGES

SEARCH CHARGES

DISPLAY CHARGES

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 3.06 | 16.81 |
| 0.54 | 3.00 |
| 147.75 | 303.94 |
| 0.00 | 7.96 |

CAPLUS FEE (5%)

| | |
|--------|--------|
| 151.35 | 331.71 |
| 0.00 | 0.40 |

FULL ESTIMATED COST

| | |
|--------|--------|
| 151.35 | 332.11 |
|--------|--------|

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 0.00 | -1.30 |

IN FILE 'REGISTRY' AT 14:06:52 ON 11 MAR 2003

=>

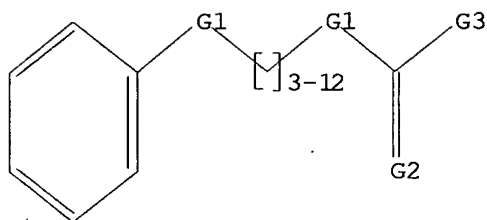
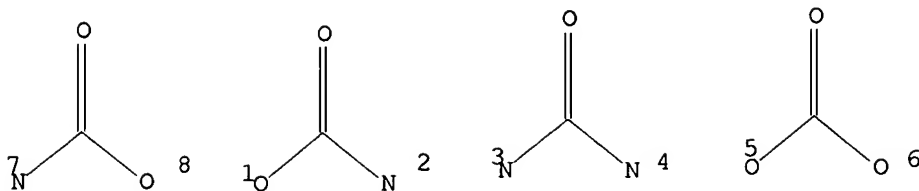
Uploading 10025947 rce first action 2nd.str

L15 STRUCTURE UPLOADED

=> d l15

L15 HAS NO ANSWERS

L15 STR



G1 CH₂,O,S,N, [01-02], [03-04], [05-06], [07-08]

G2 O, S

G3 OH, SH

Structure attributes must be viewed using STN Express query preparation.

=> search l15 sss sam

SAMPLE SEARCH INITIATED 14:10:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 0

L16 0 SEA SSS SAM L15

=> logoff hold

COST IN U.S. DOLLARS

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |
| 153.75 | 334.51 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |
| 0.00 | -1.30 |

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 14:10:50 ON 11 MAR 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal623paz

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 14:14:18 ON 11 MAR 2003
FILE 'REGISTRY' ENTERED AT 14:14:18 ON 11 MAR 2003
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| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 153.75 | 334.51 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.30 |

=>

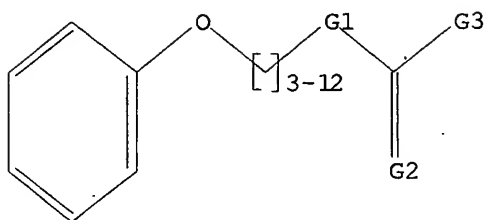
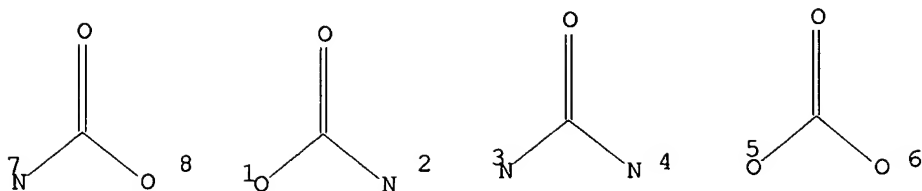
Uploading 10025947 rce first action 2nd2.str

L17 STRUCTURE UPLOADED

=> d l17

L17 HAS NO ANSWERS

L17 STR



G1 CH₂,O,S,N, [01-02],[03-04],[05-06],[07-08]

G2 O,S

G3 OH,SH

Structure attributes must be viewed using STN Express query preparation.

=> search l17 sss sam

SAMPLE SEARCH INITIATED 14:14:56 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 36404 TO ITERATE

2.7% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 716721 TO 739439

PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> search l17 sss full

FULL SEARCH INITIATED 14:15:10 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 722344 TO ITERATE

55.4% PROCESSED 400000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.07

5 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 722344 TO 722344
PROJECTED ANSWERS: 5 TO 18

L19 5 SEA SSS FUL L17

=> d scan

L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1-Hexadecanaminium, N,N,N-trimethyl-, salt with 11-phenoxyundecanoic acid
(1:1) (9CI)
MF C19 H42 N . C17 H25 O3
CM 1

$^{-}\text{O}_2\text{C}-(\text{CH}_2)_{10}-\text{OPh}$

CM 2

$\text{Me}_3^+\text{N}-(\text{CH}_2)_{15}-\text{Me}$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

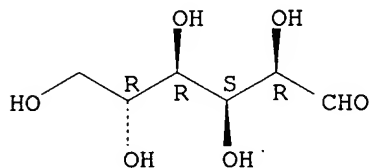
L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN D-Glucose, polymer with 7-phenoxyheptanoic acid (9CI)
MF (C13 H18 O3 . C6 H12 O6)x
CI PMS

CM 1

$\text{HO}_2\text{C}-(\text{CH}_2)_6-\text{OPh}$

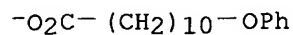
CM 2

Absolute stereochemistry.



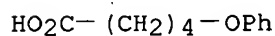
L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Undecanoic acid, 11-phenoxy-, ion(1-) (9CI)
MF C17 H25 O3
CI COM



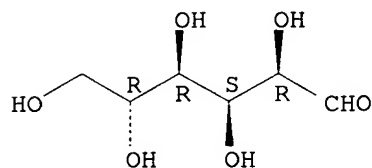
L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN D-Glucose, polymer with 5-phenoxy-pentanoic acid (9CI)
MF (C11 H14 O3 . C6 H12 O6)x
CI PMS

CM 1

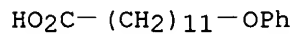


CM 2

Absolute stereochemistry.



L19 5 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Dodecanoic acid, 12-phenoxy- (9CI)
MF C18 H28 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 304.30 | 485.06 |

| | | |
|--|------------|---------|
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.30 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:18:42 ON 11 MAR 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal623paz

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 14:21:38 ON 11 MAR 2003
FILE 'REGISTRY' ENTERED AT 14:21:38 ON 11 MAR 2003
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| | | |
|----------------------|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 304.30 | 485.06 |

| | | |
|--|------------|---------|
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.30 |

=>

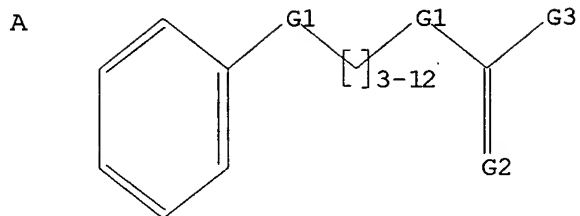
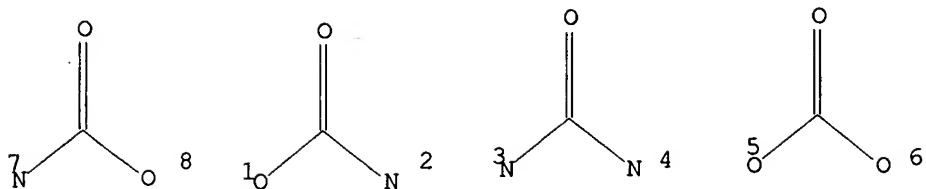
Uploading 10025947 rce first action 2nd2.str

L20 STRUCTURE UPLOADED

=> d 120

L20 HAS NO ANSWERS

L20 STR



G1 CH₂,O,S,N, [01-02], [03-04], [05-06], [07-08]

G2 O,S

G3 OH,SH

Structure attributes must be viewed using STN Express query preparation.

=> search l20 sss sam

SAMPLE SEARCH INITIATED 14:22:14 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 378773 TO ITERATE

0.3% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 0

L21 0 SEA SSS SAM L20

=>

=>

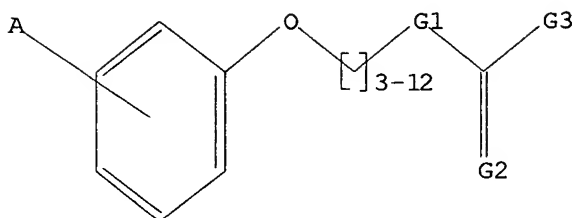
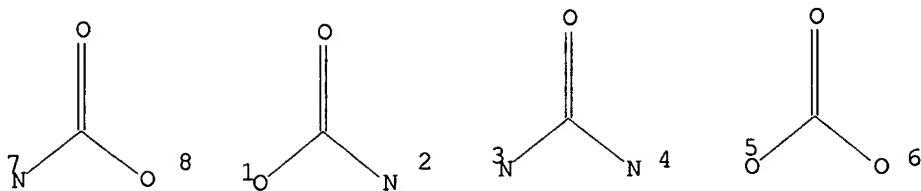
Uploading 10025947 rce first action 2nd2.str

L22 STRUCTURE UPLOADED

=> d l22

L22 HAS NO ANSWERS

L22 STR



G1 CH₂,O,S,N, [01-02], [03-04], [05-06], [07-08]

G2 O,S

G3 OH,SH

Structure attributes must be viewed using STN Express query preparation.

=> search l22 sss sam

SAMPLE SEARCH INITIATED 14:24:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 36403 TO ITERATE

2.7% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

2 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 716701 TO 739419

PROJECTED ANSWERS: 945 TO 1967

L23 2 SEA SSS SAM L22

=> d scan

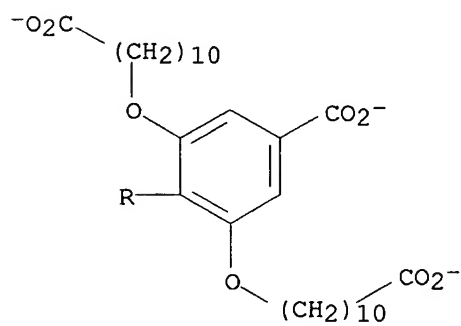
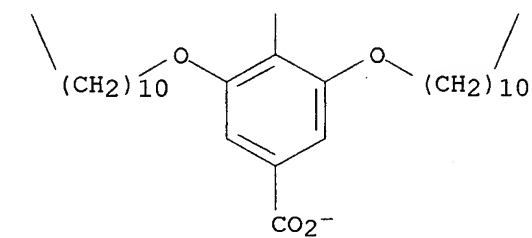
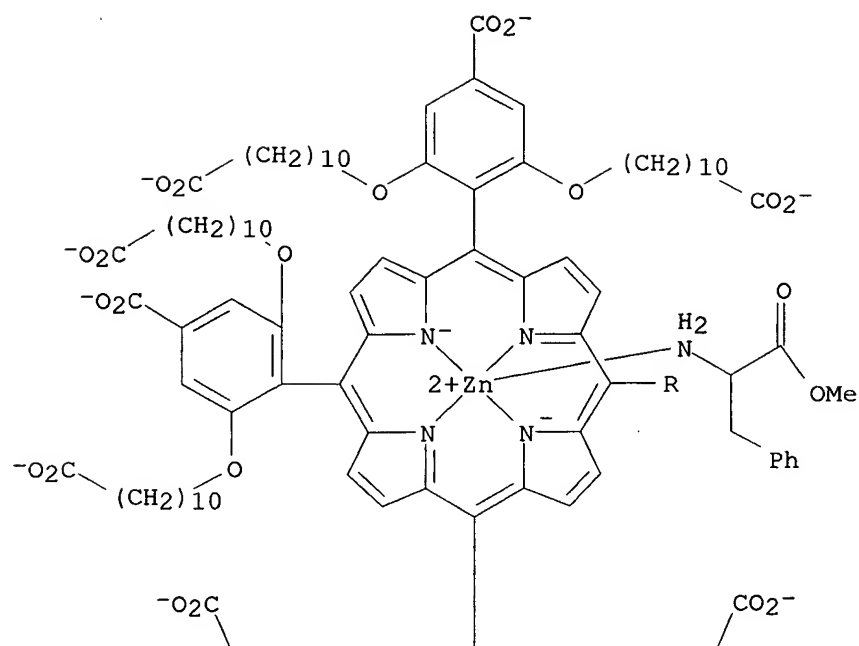
L23 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Zincate(12-), (methyl

L-phenylalaninate-.kappa.N) [[4,4',4'',4'''-(21H,23H-

porphine-5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)te
trakis[3,5-bis[(10-carboxydecyl)oxy]benzoato]](14-)]-, dodecapotassium,
(SP-5-31)-(9CI)

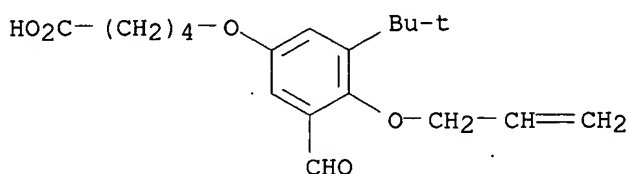
MF C146 H189 N5 O34 Zn . 12 K



12 K⁺

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L23 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[3-(1,1-dimethylethyl)-5-formyl-4-(2-propenyloxy)phenoxy]- (9CI)
 MF C19 H26 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l22 sss full
 FULL SEARCH INITIATED 14:24:48 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 722338 TO ITERATE

55.4% PROCESSED 400000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.12

1188 ANSWERS

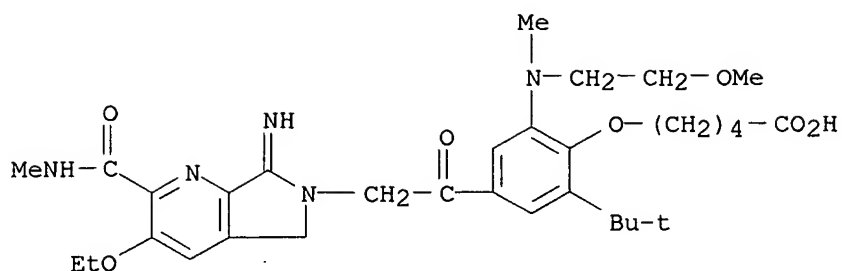
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 722338 TO 722338
 PROJECTED ANSWERS: 2007 TO 2283

L24 1188 SEA SSS FUL L22

=> d scan

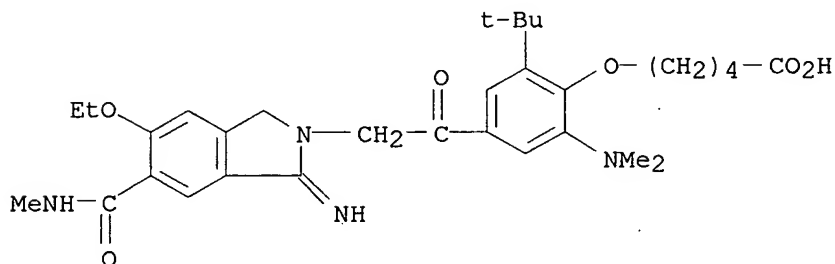
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(1,1-dimethylethyl)-4-[[3-ethoxy-5,7-dihydro-7-imino-2-[(methylamino)carbonyl]-6H-pyrrolo[3,4-b]pyridin-6-yl]acetyl]-6-[(2-methoxyethyl)methylamino]phenoxy]-, monohydrobromide (9CI)
 MF C32 H45 N5 O7 . Br H



● HBr

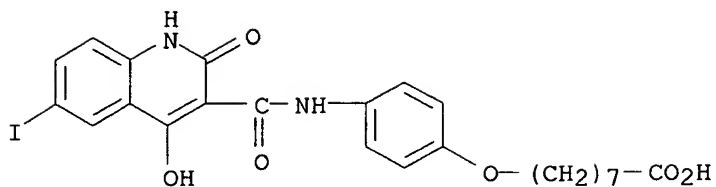
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[2-(dimethylamino)-6-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]phenoxy]-, monohydrobromide (9CI)
 MF C31 H42 N4 O6 . Br H



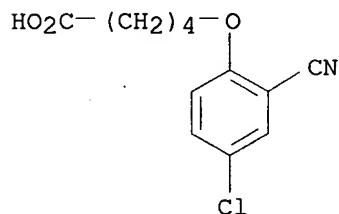
● HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-[4-[[[(1,2-dihydro-4-hydroxy-6-iodo-2-oxo-3-quinolinyl)carbonyl]amino]phenoxy]]- (9CI)
 MF C24 H25 I N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

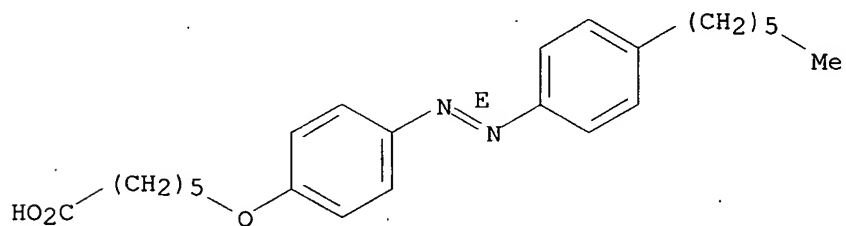
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-(4-chloro-2-cyanophenoxy)- (9CI)
 MF C12 H12 Cl N O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[4-[(1E)-(4-hexylphenyl)azo]phenoxy]- (9CI)
 MF C24 H32 N2 O3

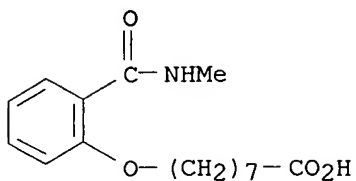
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS

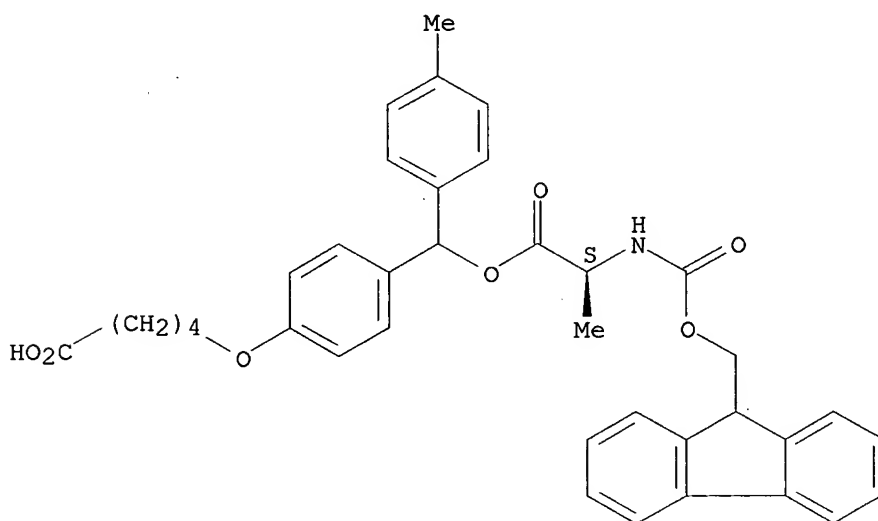
IN Octanoic acid, 8-[2-[(methylamino)carbonyl]phenoxy]- (9CI)
 MF C16 H23 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

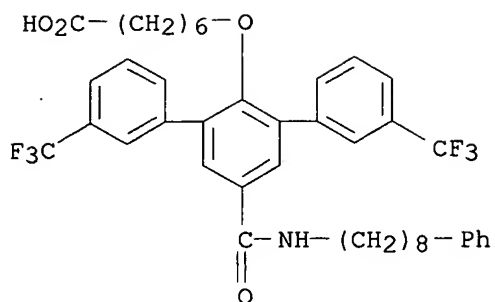
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN L-Alanine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-, [4-(4-
 carboxybutoxy)phenyl] (4-methylphenyl)methyl ester (9CI)
 MF C37 H37 N O7

Absolute stereochemistry.



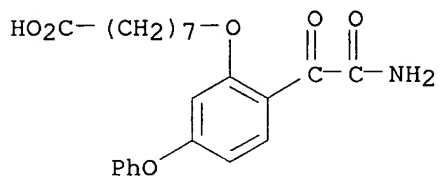
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Heptanoic acid, 7-[[5'-[[[(8-phenyloctyl)amino]carbonyl]-3,3''-
 bis(trifluoromethyl)[1,1':3',1''-terphenyl]-2''-yl]oxy]- (9CI)
 MF C42 H45 F6 N O4



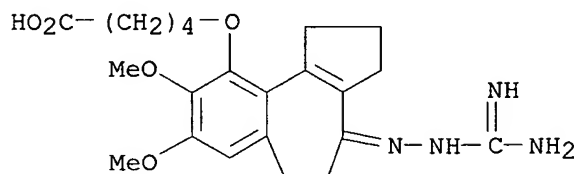
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-[2-(aminooxoacetyl)-5-phenoxyphenoxy]- (9CI)
 MF C22 H25 N O6



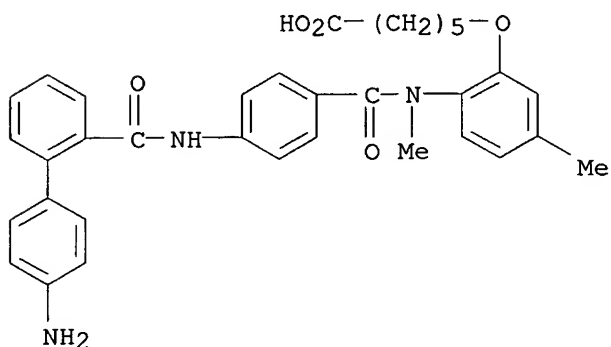
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[4-[(aminooximino)hydrazono]-1,2,3,4,5,6-hexahydro-
 8,9-dimethoxybenz[e]azulen-10-yl]oxy]- (9CI)
 MF C22 H30 N4 O5



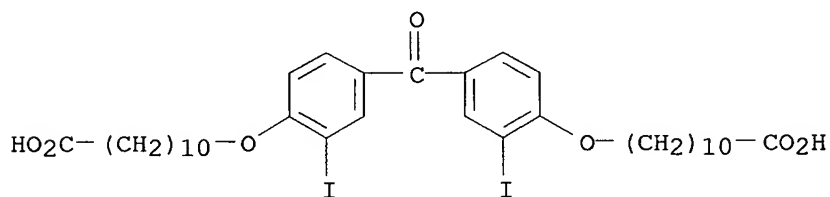
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[2-[[4-[[[4'-amino[1,1'-biphenyl]-2-yl)carbonyl]amino]benzoyl]methylamino]-5-methylphenoxy]- (9CI)
 MF C34 H35 N3 O5



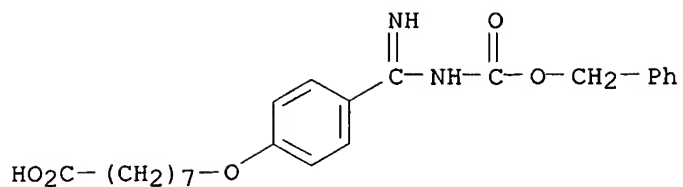
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Undecanoic acid, 11,11'-[carbonylbis[(2-iodo-4,1-phenylene)oxy]]bis- (9CI)
 MF C35 H48 I2 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

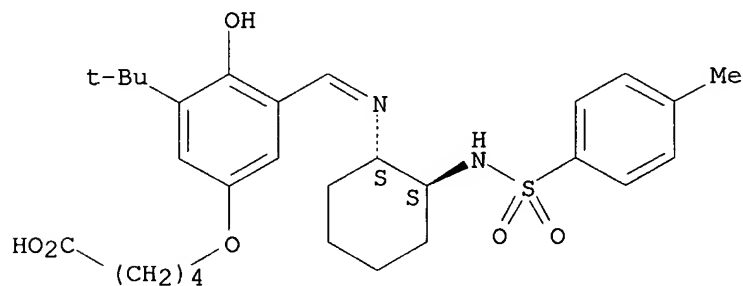
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-[4-[imino[(phenylmethoxy)carbonyl]amino]methyl]phenoxy]- (9CI)
 MF C23 H28 N2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

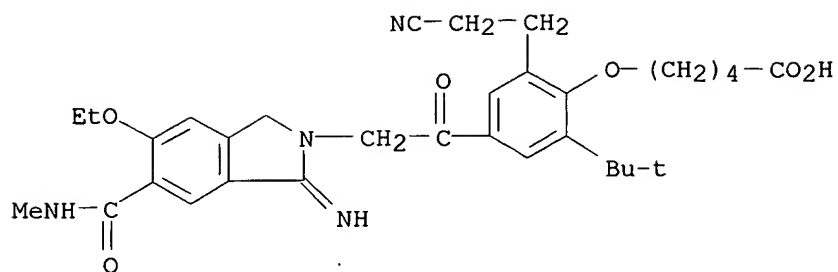
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[3-(1,1-dimethylethyl)-4-hydroxy-5-[[[(1S,2S)-2-[[4-methylphenyl)sulfonyl]amino]cyclohexyl]imino]methyl]phenoxy]- (9CI)
 MF C29 H40 N2 O6 S

Absolute stereochemistry.
 Double bond geometry unknown.



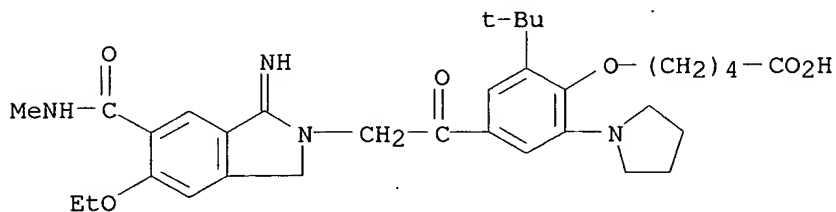
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(2-cyanoethyl)-6-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-dihydro-1-imino-6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]phenoxy]-, monohydrobromide (9CI)
 MF C32 H40 N4 O6 . Br H



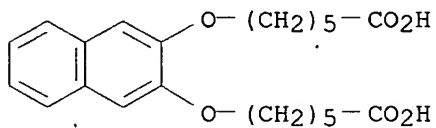
● HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(1,1-dimethylethyl)-4-[[5-ethoxy-1,3-dihydro-1-imino-
 6-[(methylamino)carbonyl]-2H-isoindol-2-yl]acetyl]-6-(1-
 pyrrolidinyl)phenoxy]- (9CI)
 MF C33 H44 N4 O6
 CI COM



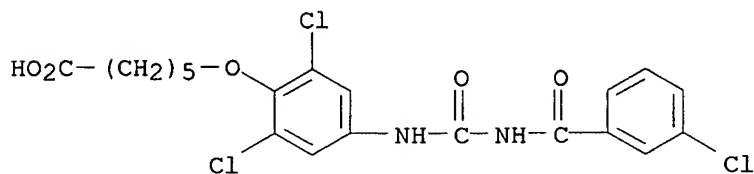
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6,6'-[2,3-naphthalenediylbis(oxy)]bis- (9CI)
 MF C22 H28 O6



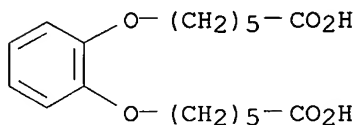
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[2,6-dichloro-4-[[[(3-chlorobenzoyl)amino]carbonyl]amino]
 phenoxy]- (9CI)
 MF C20 H19 Cl3 N2 O5
 CI COM



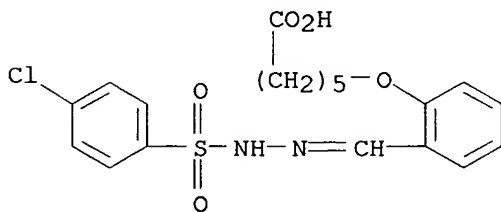
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6,6'-[1,2-phenylenebis(oxy)]bis- (9CI)
 MF C18 H26 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

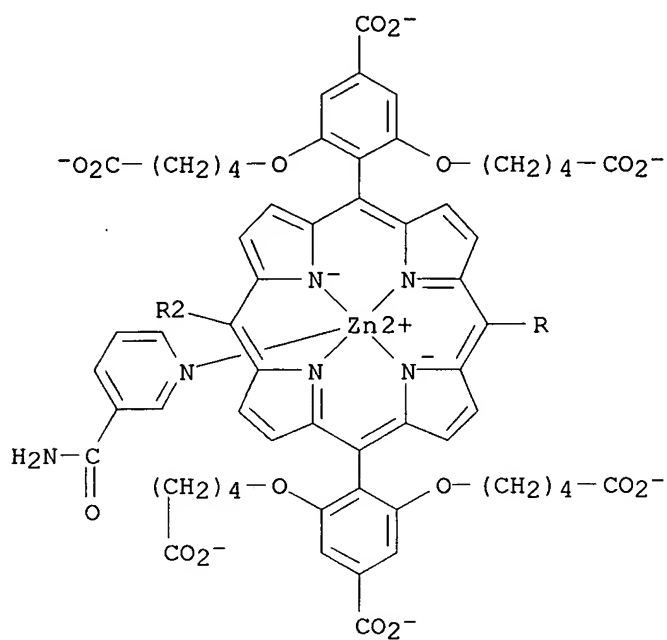
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[2-[[[(4-chlorophenyl)sulfonyl]hydrazono]methyl]phenoxy]-
 (9CI)
 MF C19 H21 Cl N2 O5 S

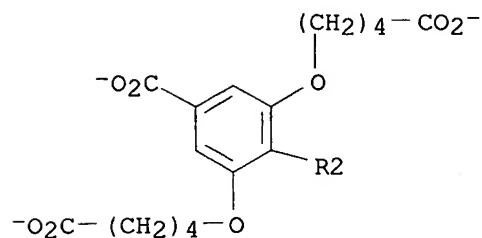
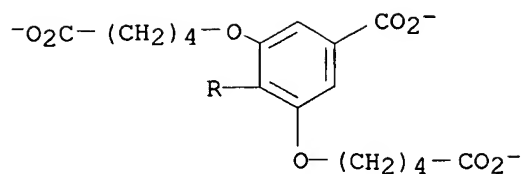


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Zincate(12-), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl-
 .kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)tetrakis[3,5-bis(4-
 carboxybutoxy)benzoato]](14-)](3-pyridinecarboxamide-.kappa.N1)-,
 dodecapotassium, (SP-5-21)-(9CI)
 MF C94 H86 N6 O33 Zn . 12 K
 CI CCS

PAGE 1-A

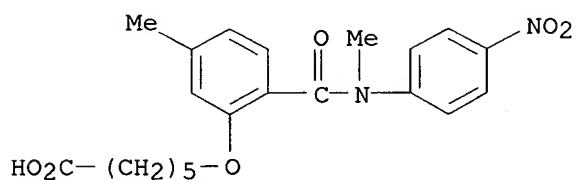




●12 K⁺

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid,
 6-[5-methyl-2-[[methyl(4-nitrophenyl)amino]carbonyl]phenoxy
]- (9CI)
 MF C21 H24 N2 O6



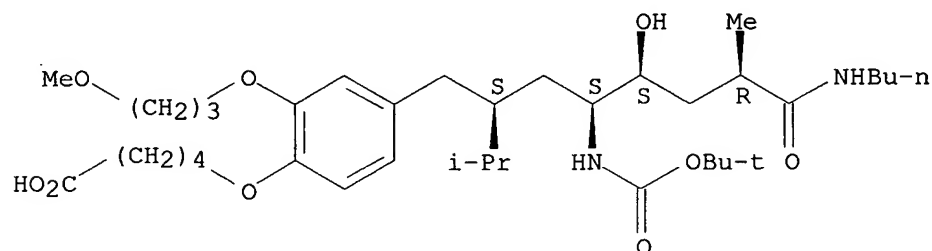
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Heptanoic acid, 7-[(5,9,10,14-tetraethyl-21-methoxy-4,15-dimethyl-8,11-
 imino-3,6:16,13-dinitrilo-1,18-benzodiazacycloeicosin-20-yl)oxy]- (9CI)
 MF C40 H49 N5 O4



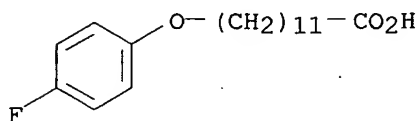
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Absolute stereochemistry.



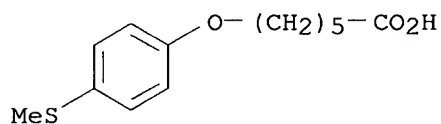
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Dodecanoic acid, 12-(4-fluorophenoxy)- (9CI)
MF C18 H27 F O3



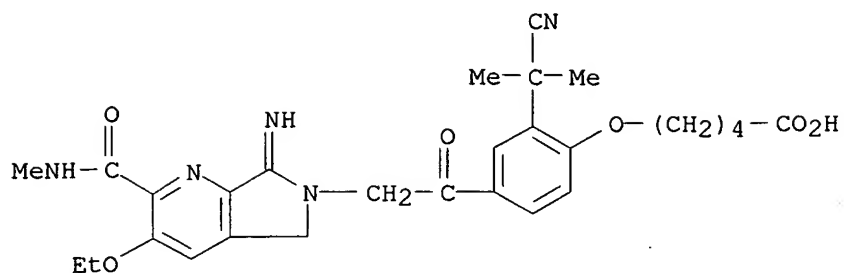
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Hexanoic acid, 6-[4-(methylthio)phenoxy]- (9CI)
MF C13 H18 O3 S



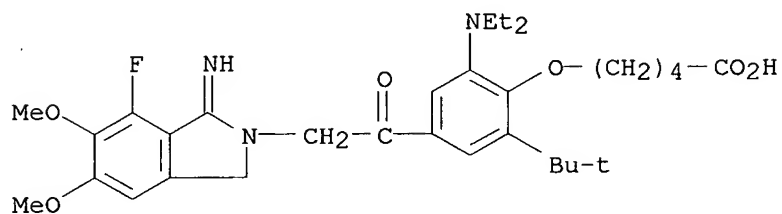
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Pentanoic acid, 5-[2-(1-cyano-1-methylethyl)-4-[[3-ethoxy-5,7-dihydro-7-imino-2-[(methylamino)carbonyl]-6H-pyrrolo[3,4-b]pyridin-6-yl]acetyl]phenoxy]-, monohydrobromide (9CI)
MF C28 H33 N5 O6 . Br H



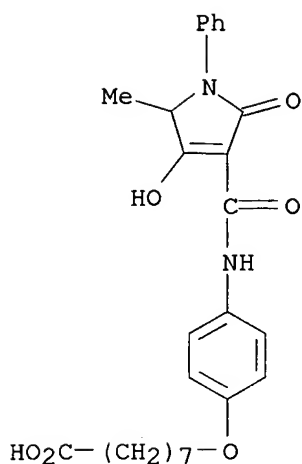
● HBr

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(diethylamino)-6-(1,1-dimethylethyl)-4-[(7-fluoro-1,3-
 dihydro-1-imino-5,6-dimethoxy-2H-isoindol-2-yl)acetyl]phenoxy]-,
 monohydrobromide (9CI)
 MF C31 H42 F N3 O6 . Br H



● HBr

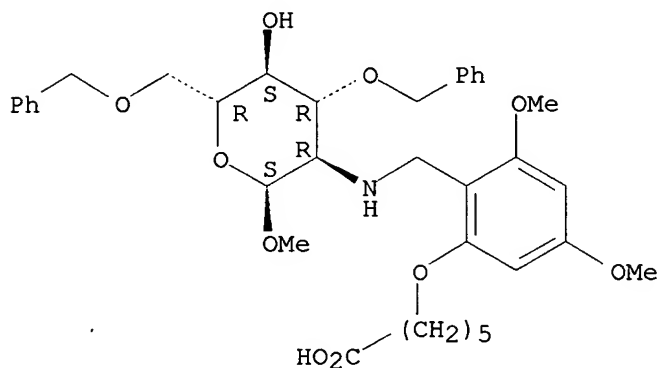
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-[4-[[[(2,5-dihydro-4-hydroxy-5-methyl-2-oxo-1-phenyl-1H-
 pyrrol-3-yl)carbonyl]amino]phenoxy]- (9CI)
 MF C26 H30 N2 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

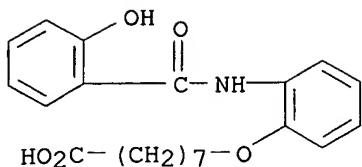
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN .alpha.-D-Glucopyranoside, methyl 2-[[[2-[(5-carboxypentyl)oxy]-4,6-
 dimethoxyphenyl]methyl]amino]-2-deoxy-3,6-bis-O-(phenylmethyl)- (9CI)
 MF C36 H47 N O10

Absolute stereochemistry.



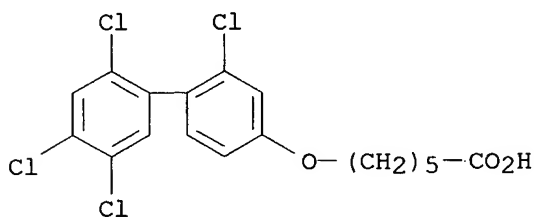
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-[2-[(2-hydroxybenzoyl)amino]phenoxy]- (9CI)
 MF C21 H25 N O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[(2,2',4',5'-tetrachloro[1,1'-biphenyl]-4-yl)oxy]- (9CI)
 MF C18 H16 Cl4 O3

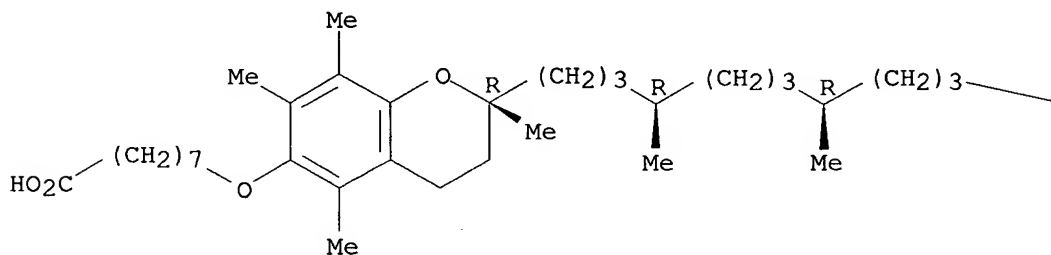


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid,
 8-[(2R)-3,4-dihydro-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-2H-1-benzopyran-6-yl]oxy]- (9CI)
 MF C37 H64 O4

Absolute stereochemistry.

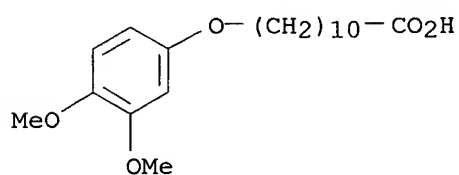
PAGE 1-A



—CHMe₂

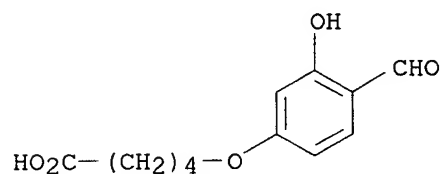
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Undecanoic acid, 11-(3,4-dimethoxyphenoxy)- (9CI)
 MF C19 H30 O5



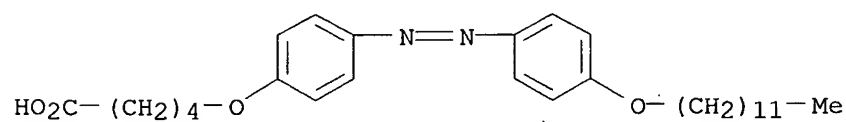
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

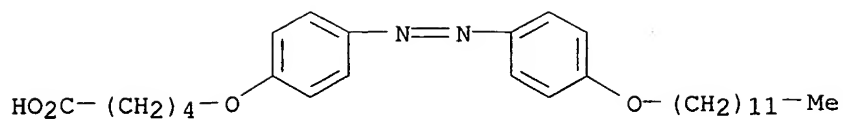
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-(4-formyl-3-hydroxyphenoxy)- (9CI)
 MF C12 H14 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[4-[[4-(dodecyloxy)phenyl]azo]phenoxy]- (9CI)
 MF C29 H42 N2 O4

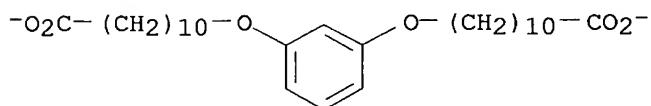




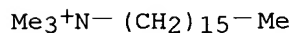
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 1-Hexadecanaminium, N,N,N-trimethyl-, salt with 11,11'-[1,3-phenylenebis(oxy)]bis[undecanoic acid] (2:1) (9CI)
 MF C28 H44 O6 . 2 C19 H42 N

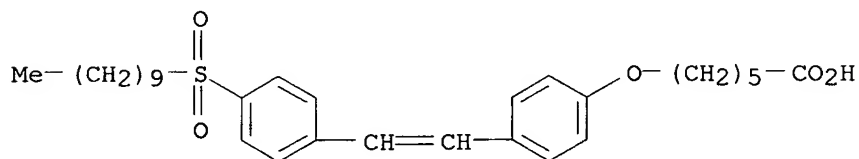
CM 1



CM 2



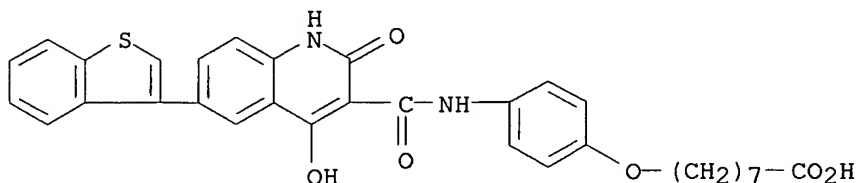
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[4-[2-[4-(decylsulfonyl)phenyl]ethenyl]phenoxy]- (9CI)
 MF C30 H42 O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

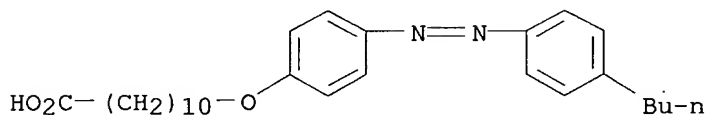
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Dodecanoic acid, 12-[2-[(3-carboxypropyl)thio]phenoxy]- (9CI)
 MF C22 H34 O5 S

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid,
 8-[4-[[(6-benzo[b]thien-3-yl-1,2-dihydro-4-hydroxy-2-oxo-3-
 quinolinyl)carbonyl]amino]phenoxy]- (9CI)
 MF C32 H30 N2 O6 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

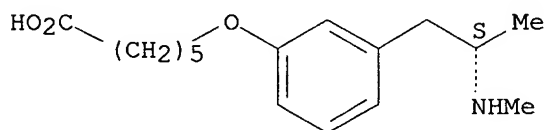
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Undecanoic acid, 11-[4-[(4-butylphenyl)azo]phenoxy]- (9CI)
 MF C27 H38 N2 O3
 CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

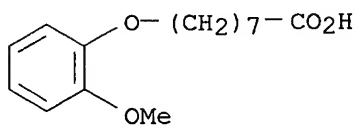
L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Hexanoic acid, 6-[3-[(2S)-2-(methylamino)propyl]phenoxy]-, hydrochloride
 (9CI)
 MF C16 H25 N O3 . Cl H

Absolute stereochemistry.



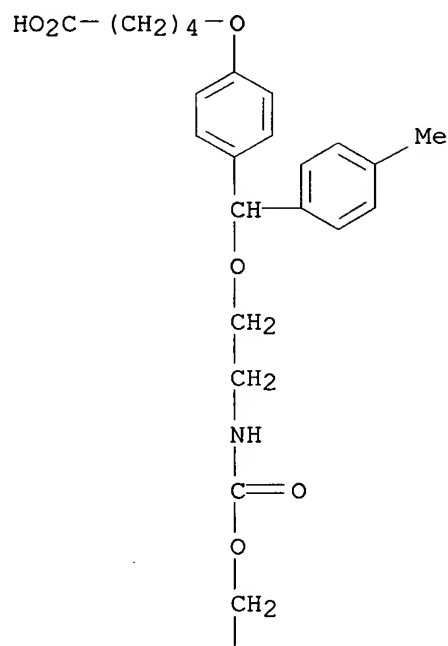
HCl

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-(2-methoxyphenoxy)- (9CI)
 MF C15 H22 O4

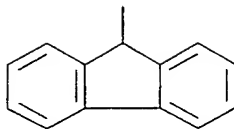


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[4-[[2-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]ethoxy](4-methylphenyl)methyl]phenoxy]- (9CI)
 MF C36 H37 N O6

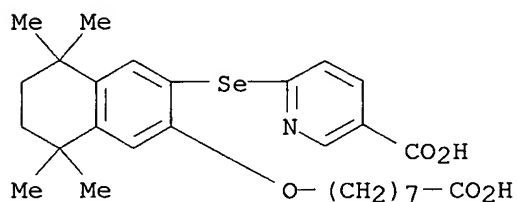


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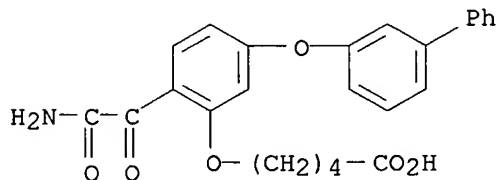
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 3-Pyridinecarboxylic acid,
 6-[[3-[(7-carboxyheptyl)oxy]-5,6,7,8-tetrahydro-
 5,5,8,8-tetramethyl-2-naphthalenyl]seleno]- (9CI)
 MF C28 H37 N O5 Se



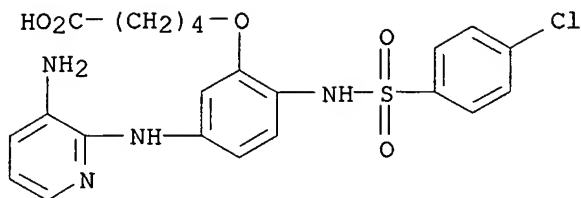
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid,
 5-[2-(aminooxoacetyl)-5-([1,1'-biphenyl]-3-yloxy)phenoxy]-
 (9CI)
 MF C25 H23 N O6



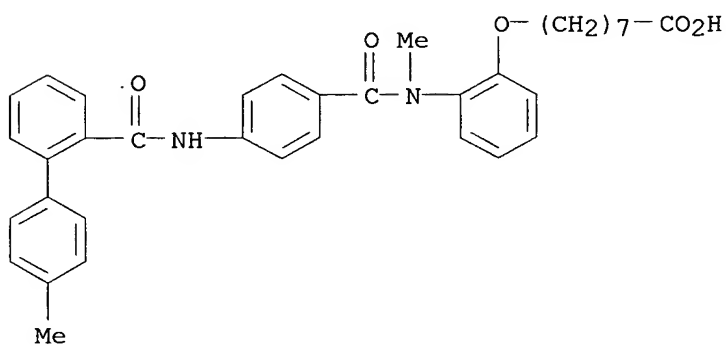
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Pentanoic acid, 5-[5-[(3-amino-2-pyridinyl)amino]-2-[[4-
 chlorophenyl)sulfonyl]amino]phenoxy]- (9CI)
 MF C22 H23 Cl N4 O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L24 1188 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Octanoic acid, 8-[2-[methyl[4-[[(4'-methyl[1,1'-biphenyl]-2-yl)carbonyl]amino]benzoyl]amino]phenoxy]- (9CI)
 MF C36 H38 N2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> save temp l24 histcmpds2a/
 HISTCMPDS2A/ IS NOT A VALID SAVED NAME
 Enter the name you wish to use for the saved query,
 answer set, or L-number list. The name must:

1. Begin with a letter,
2. Have 1-12 characters,
3. Contain only letters (A-Z) and numbers (0-9),
4. End with /Q for a query (search profile, structure, or screen set), /A for an answer set, or /L for an L-number list.
5. Not already be in use as a saved name,

6. Not be END, SAV, SAVE, SAVED
 7. Not have the form of an L-number (Lnnn).
 ENTER NAME OR (END):histcmpds2/a
 ANSWER SET L24 HAS BEEN SAVED AS 'HISTCMPDS2/A'

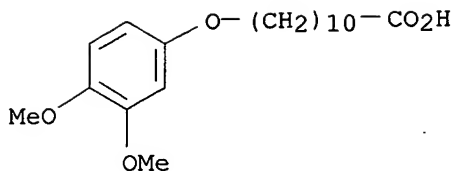
=> e Hexanoic acid, 6,6'-(1,2-phenylenebis(oxy))bis-/cn
 MISMATCHED QUOTE IN EXPAND TERM
 Quotation marks (or apostrophes) must be used in pairs,
 one before and one after the expression you are setting
 off or masking.

=> e Undecanoic acid, 11-(3,4-dimethoxyphenoxy)-/cn
 E1 1 UNDECANOIC ACID, 11-(2-THIAZOLIN-2-YLAMINO)-, PICRATE/CN
 E2 1 UNDECANOIC ACID, 11-(3,4-DIHYDROXYPHENYL)-, METHYL ESTER/CN
 E3 1 --> UNDECANOIC ACID, 11-(3,4-DIMETHOXYPHENOXY)-/CN
 E4 1 UNDECANOIC ACID, 11-(3,4-XYLYL)-, METHYL ESTER/CN
 E5 1 UNDECANOIC ACID,
 11-(3-(((2,2-DIMETHYL-1,3-DIOXOLAN-4-YL)ME
 THOXY)HYDROXYPHOSPHINYL)OXY)-2-METHOXYPROPOXY)-,
 (S-(R*,S*))
 -/CN
 E6 1 UNDECANOIC ACID,
 11-(3-((HYDROXY(2-(4-NITROPHENYL)ETHOXY)PHO
 SPHINYL)OXY)-2-METHOXYPROPOXY)-, (R)-/CN
 E7 1 UNDECANOIC ACID, 11-(3-(1-ADAMANTYL)UREIDO)-/CN
 E8 1 UNDECANOIC ACID, 11-(3-(1-ADAMANTYL)UREIDO)-,
 3-(DIMETHYLAMI
 NO)PROPYL ESTER/CN
 E9 1 UNDECANOIC ACID, 11-(3-(1-ADAMANTYL)UREIDO)-, ETHYL
 ESTER/CN
 E10 1 UNDECANOIC ACID,
 11-(3-(10,15,20-TRIS(4-METHYLPHENYL)-21H,23
 H-PORPHIN-5-YL)PHENOXY)-/CN
 E11 1 UNDECANOIC ACID,
 11-(3-(10,15,20-TRIS(4-METHYLPHENYL)-21H,23
 H-PORPHIN-5-YL)PHENOXY)-, METHYL ESTER/CN
 E12 1 UNDECANOIC ACID,
 11-(3-(2-(3-(HYDROXYMETHYL)-4-OXO-2-OXETANY
 L)ETHYL)PHENOXY)-, METHYL ESTER, TRANS-/CN

=> e3
 L25 1 "UNDECANOIC ACID, 11-(3,4-DIMETHOXYPHENOXY)-"/CN

=> d 125

L25 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
 RN 227291-94-3 REGISTRY
 CN **Undecanoic acid, 11-(3,4-dimethoxyphenoxy)- (9CI)** (CA INDEX
 NAME)
 FS 3D CONCORD
 MF C19 H30 O5
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file ca[plus
'CAOLUS' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'REGISTRY'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

| | | |
|--|------------------|---------------|
| => file caplus | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 463.15 | 643.91 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.30 |

FILE 'CAPLUS' ENTERED AT 14:29:42 ON 11 MAR 2003
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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11
FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 125
L26 1 L25

=> d 126 ti fbib abs

L26 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
TI Preparation of arylalkanoic acids and analogs as fibroblast growth factor
receptor antagonists
AN 1999:388146 CAPLUS
DN 131:44430
TI Preparation of arylalkanoic acids and analogs as fibroblast growth factor
receptor antagonists
IN Chan, Ming Fai; Balaji, Vitukudi Narayanaiyengar; Ramnarayan,
Kalyanaraman; Schove, Laura; Castillo, Rosario Silvestre; Kois, Adam
PA Eisai Co., Ltd., Japan
SO PCT Int. Appl., 155 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| PI | WO 9929640 | A2 | 19990617 | WO 1998-US25789 | 19981204 |
| | WO 2000029640 | A3 | 20000113 | | |
| | W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, | | | | |
| TM | RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | | | | US 1997-986248 | 19971205 |
| | | | | US 1998-79343 | 19980515 |
| | AU 9919037 | A1 | 19990628 | AU 1999-19037 | 19981204 |
| | | | | US 1997-986248 | 19971205 |
| | | | | US 1998-79343 | 19980515 |
| | | | | WO 1998-US25789 | 19981204 |
| OS | MARPAT 131:44430 | | | | |
| AB | RZZ1R1 [I; R = (un)substituted (hetero)aryl; R1 = CO2H, B(OH)2, SO3H, P(O)(OH)2; Z = bond, O, NH, CO, alkenylene, etc.; Z1 = alkylene, arylene, O, NH, etc.] were prepd. Thus, 4-IC6H4OCH2CO2H was condensed with PhC.tplbond.CH to give 4-(PhC.tplbond.C)C6H4OCH2CO2H. Data for biol. activity of I were given. | | | | |

=> fil;e reg

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 4.08 | 647.99 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| -0.65 | -1.95 |

CA SUBSCRIBER PRICE

FILE 'HOME' ENTERED AT 14:32:16 ON 11 MAR 2003

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

The EXPAND command is used to look at the index in a file which has an index. This file does not have an index.

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.21 | 648.20 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | 0.00 | -1.95 |

FILE 'REGISTRY' ENTERED AT 14:32:24 ON 11 MAR 2003
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STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7
DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNnote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e Octanoic acid, 8-(2-methoxyphenoxy)-/cn

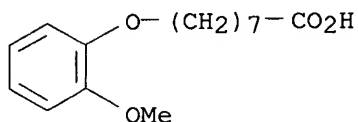
| | | |
|-----|-------|--|
| E1 | 1 | OCTANOIC ACID, 8-(2-ISOINDOLINYL)-/CN |
| E2 | 1 | OCTANOIC ACID, 8-(2-METHOXYETHOXY)-/CN |
| E3 | 1 --> | OCTANOIC ACID, 8-(2-METHOXYPHENOXY)-/CN |
| E4 | 1 | OCTANOIC ACID, 8-(2-METHYLPHENOXY)-/CN |
| E5 | 1 | OCTANOIC ACID, 8-(2-NAPHTHALENYLAMINO)-8-OXO-, METHYL ESTER/ |
| | | CN |
| E6 | 1 | OCTANOIC ACID, 8-(2-NAPHTHALENYLOXY)-, ETHYL ESTER/CN |
| E7 | 1 | OCTANOIC ACID, 8-(2-NAPHTHALENYLTHIO)-2-OXO-, METHYL ESTER/C |
| | | N |
| E8 | 1 | OCTANOIC ACID, 8-(2-NAPHTHOYL)-/CN |
| E9 | 1 | OCTANOIC ACID, 8-(2-NITROPHENOXY)-/CN |
| E10 | 1 | OCTANOIC ACID, 8-(2-OXOCYCLOPENTYLIDENE)-/CN |
| E11 | 1 | OCTANOIC ACID, 8-(2-OXOCYCLOPENTYLIDENE)-, METHYL ESTER/CN |
| E12 | 1 | OCTANOIC ACID, 8-(2-PROPENYLOXY)-/CN |

=> e3

L27 1 "OCTANOIC ACID, 8-(2-METHOXYPHENOXY)-"/CN

=> d 127

L27 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
 RN 338994-29-9 REGISTRY
 CN Octanoic acid, 8-(2-methoxyphenoxy)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C15 H22 O4
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus

| | | |
|----------------------|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 6.30 | 654.50 |

| | | |
|--|------------------|---------------|
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.95 |

FILE 'CAPLUS' ENTERED AT 14:32:49 ON 11 MAR 2003
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FILE COVERS 1907 - 11 Mar 2003 VOL 138 ISS 11
 FILE LAST UPDATED: 10 Mar 2003 (20030310/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 127

L28 1 L27

=> d 128 ti fbib abs

L28 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

TI Preparation of phenoxyalkanoic acids as drug delivery agents

AN 2001:338472 CAPLUS

DN 134:353172

TI Preparation of phenoxyalkanoic acids as drug delivery agents

IN Leone-Bay, Andrea; Kraft, Kelly; Moye-Sherman, Destardi; Gschneidner, David; Boyd, Maria A. P.; Liu, Puchun; Tang, Pinwah; Liao, Jun; Smarth, John E.; Freeman, John J., Jr.

PA Emisphere Technologies, Inc., USA

SO PCT Int. Appl., 107 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|--|----------|------------------|----------|
| PI | WO 2001032596 | A1 | 20010510 | WO 2000-US30662 | 20001106 |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| | | | | US 1999-163806PP | 19991105 |
| | | | | US 2000-231836PP | 20000906 |
| | | | | US 2000-237233PP | 20001002 |
| | BR 2000015567 | A | 20020716 | BR 2000-15567 | 20001106 |
| | | | | US 1999-163806PP | 19991105 |
| | | | | US 2000-231836PP | 20000906 |
| | | | | US 2000-237233PP | 20001002 |
| | | | | WO 2000-US30662W | 20001106 |
| | EP 1226104 | A1 | 20020731 | EP 2000-979142 | 20001106 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | |
| | | | | US 1999-163806PP | 19991105 |
| | | | | US 2000-231836PP | 20000906 |
| | | | | US 2000-237233PP | 20001002 |
| | | | | WO 2000-US30662W | 20001106 |

PATENT FAMILY INFORMATION:

FAN 2001:338308

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---------------|--|----------|-----------------|----------|
| PI | WO 2001032130 | A2 | 20010510 | WO 2000-US41960 | 20001106 |
| | WO 2001032130 | A3 | 20020314 | | |
| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| | RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |

| | | |
|---|-------------|---------------------------|
| | | US 1999-163806PP 19991105 |
| | | US 2000-231836PP 20000906 |
| | | US 2000-237233PP 20001002 |
| AU 2001026223 | A5 20010514 | AU 2001-26223 20001106 |
| | | US 1999-163806PP 19991105 |
| | | US 2000-231836PP 20000906 |
| | | US 2000-237233PP 20001002 |
| | | WO 2000-US41960W 20001106 |
| EP 1226109 | A2 20020731 | EP 2000-989761 20001106 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | |
| | | US 1999-163806PP 19991105 |
| | | US 2000-231836PP 20000906 |
| | | US 2000-237233PP 20001002 |
| | | WO 2000-US41960W 20001106 |

OS MARPAT 134:353172

AB R1OZ1Z2CO2H [I; R1 = (un)substituted Ph; Z1 = (heteroatom-interrupted) alk(en)ylene or (hetero)arylene; Z2 = bond, (hydroxy)arylene, haloarylene]

were prepd. Thus, 2-(HO)C6H4OCH2Ph was etherified by Br(CH2)6CO2Et and the product deprotected to give 2-(HO)C6H4O(CH2)6CO2H. Data for drug delivery activity of I were given.

RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

| | | |
|--|------------|---------|
| => logoff hold | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 10.12 | 664.62 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -0.65 | -2.60 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:35:14 ON 11 MAR 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal623paz

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

| | |
|---------------|--|
| NEWS 1 | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 Apr 08 | "Ask CAS" for self-help around the clock |
| NEWS 3 Apr 09 | BEILSTEIN: Reload and Implementation of a New Subject Area |
| NEWS 4 Apr 09 | ZDB will be removed from STN |
| NEWS 5 Apr 19 | US Patent Applications available in IFICDB, IFIPAT, and IFIUDB |

NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS

NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER

NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available

NEWS 9 Jun 03 New e-mail delivery for search results now available

NEWS 10 Jun 10 MEDLINE Reload

NEWS 11 Jun 10 PCTFULL has been reloaded

NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment

NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
saved answer sets no longer valid

NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY

NEWS 15 Jul 30 NETFIRST to be removed from STN

NEWS 16 Aug 08 CANCERLIT reload

NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN

NEWS 18 Aug 08 NTIS has been reloaded and enhanced

NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN

NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded

NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded

NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced

NEWS 23 Sep 03 JAPIO has been reloaded and enhanced

NEWS 24 Sep 16 Experimental properties added to the REGISTRY file

NEWS 25 Sep 16 CA Section Thesaurus available in CAPLUS and CA

NEWS 26 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985

NEWS 27 Oct 21 EVENTLINE has been reloaded

NEWS 28 Oct 24 BEILSTEIN adds new search fields

NEWS 29 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN

NEWS 30 Oct 25 MEDLINE SDI run of October 8, 2002

NEWS 31 Nov 18 DKILIT has been renamed APOLLIT

NEWS 32 Nov 25 More calculated properties added to REGISTRY

NEWS 33 Dec 02 TIBKAT will be removed from STN

NEWS 34 Dec 04 CSA files on STN

NEWS 35 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date

NEWS 36 Dec 17 TOXCENTER enhanced with additional content

NEWS 37 Dec 17 Adis Clinical Trials Insight now available on STN

NEWS 38 Dec 30 ISMEC no longer available

NEWS 39 Jan 13 Indexing added to some pre-1967 records in CA/CAPLUS

NEWS 40 Jan 21 NUTRACEUT offering one free connect hour in February 2003

NEWS 41 Jan 21 PHARMAML offering one free connect hour in February 2003

NEWS 42 Jan 29 Simultaneous left and right truncation added to COMPENDEX,
ENERGY, INSPEC

NEWS 43 Feb 13 CANCERLIT is no longer being updated

NEWS 44 Feb 24 METADEX enhancements

NEWS 45 Feb 24 PCTGEN now available on STN

NEWS 46 Feb 24 TEMA now available on STN

NEWS 47 Feb 26 NTIS now allows simultaneous left and right truncation

NEWS 48 Feb 26 PCTFULL now contains images

NEWS 49 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results

NEWS EXPRESS January 6 CURRENT WINDOWS VERSION IS V6.01a,
CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS INTER General Internet Information

NEWS LOGIN Welcome Banner and News Items

NEWS PHONE Direct Dial and Telecommunication Network Access to STN

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 07:26:13 ON 12 MAR 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 07:26:19 ON 12 MAR 2003

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STRUCTURE FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

DICTIONARY FILE UPDATES: 10 MAR 2003 HIGHEST RN 497818-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

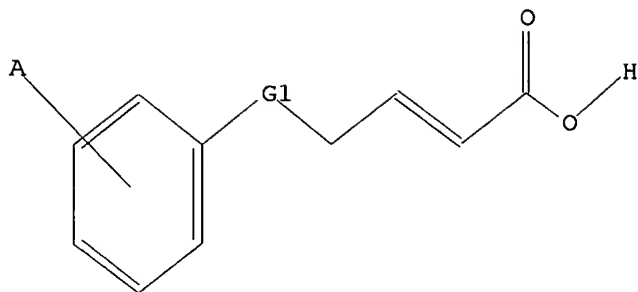
Uploading 10025947 rce first action 2nd3.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 07:26:46 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 516 TO ITERATE

100.0% PROCESSED 516 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8958 TO 11682

PROJECTED ANSWERS: 931 TO 1949

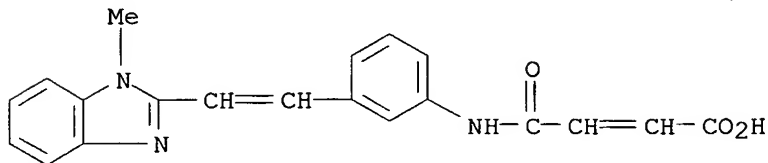
L2 50 SEA SSS SAM L1

=> d scan

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-[[3-[2-(1-methyl-1H-benzimidazol-2-yl)ethenyl]phenyl]amino]-4-oxo-, monosodium salt (9CI)

MF C20 H17 N3 O3 . Na

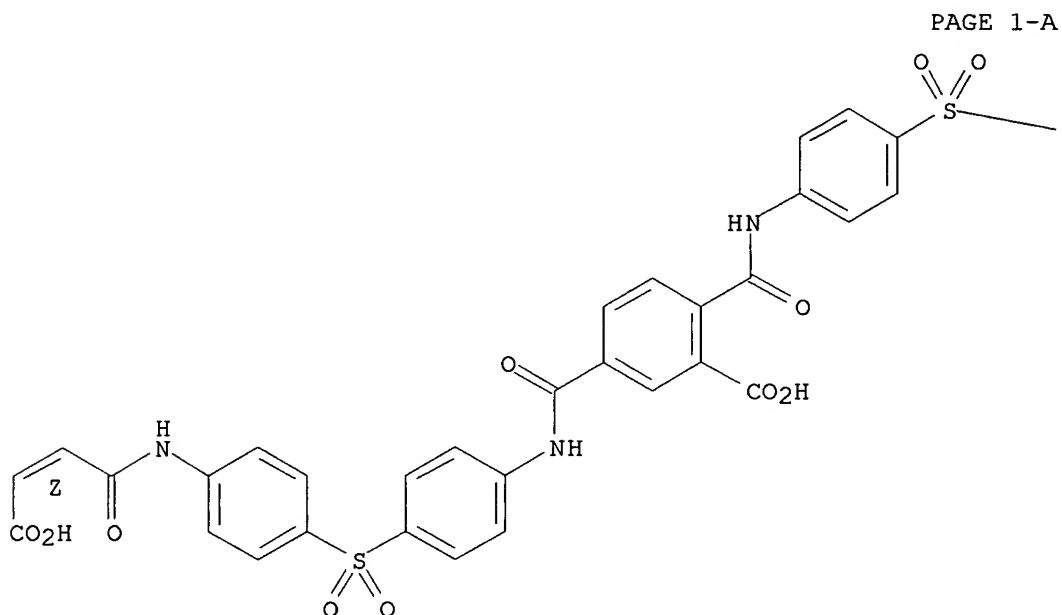


● Na

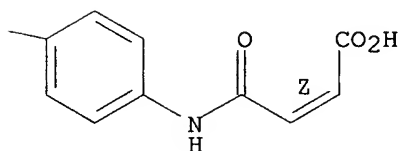
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 2,5-bis[[[4-[[4-[(3-carboxy-1-oxo-2-propenyl)amino]phenyl]sulfonyl]phenyl]amino]carbonyl]-, (Z,Z)- (9CI)
MF C41 H30 N4 O14 S2

Double bond geometry as shown.



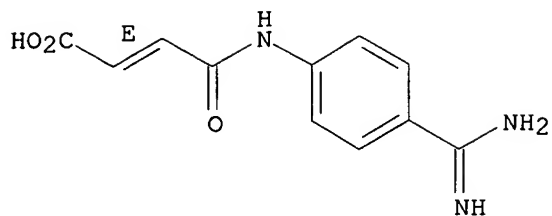
PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

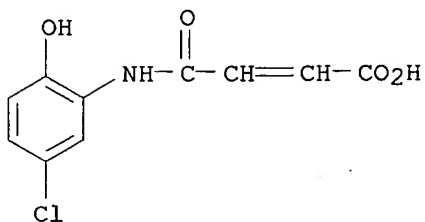
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Butenoic acid, 4-[[4-(aminoiminomethyl)phenyl]amino]-4-oxo-, (E)- (9CI)
MF C11 H11 N3 O3
CI COM

Double bond geometry as shown.



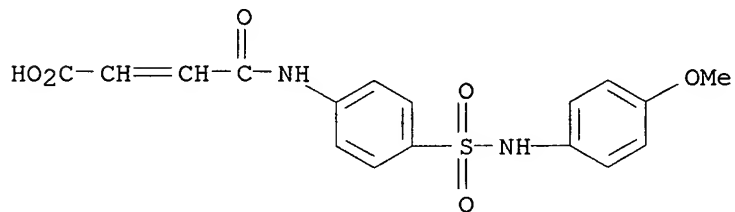
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[(5-chloro-2-hydroxyphenyl)amino]-4-oxo- (9CI)
 MF C10 H8 Cl N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

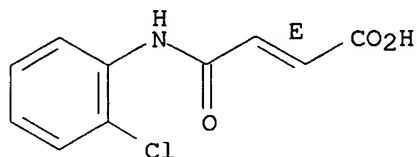
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[[4-[(4-methoxyphenyl)amino]sulfonyl]phenyl]amino]-4-oxo- (9CI)
 MF C17 H16 N2 O6 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS . REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[(2-chlorophenyl)amino]-4-oxo-, (E)- (9CI)
 MF C10 H8 Cl N O3

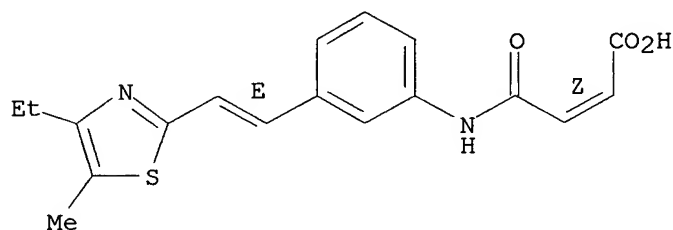
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[[3-[2-(4-ethyl-5-methyl-2-thiazolyl)ethenyl]phenyl]amino]-4-oxo-, monosodium salt, (E,Z)- (9CI)
 MF C18 H18 N2 O3 S . Na

Double bond geometry as shown.



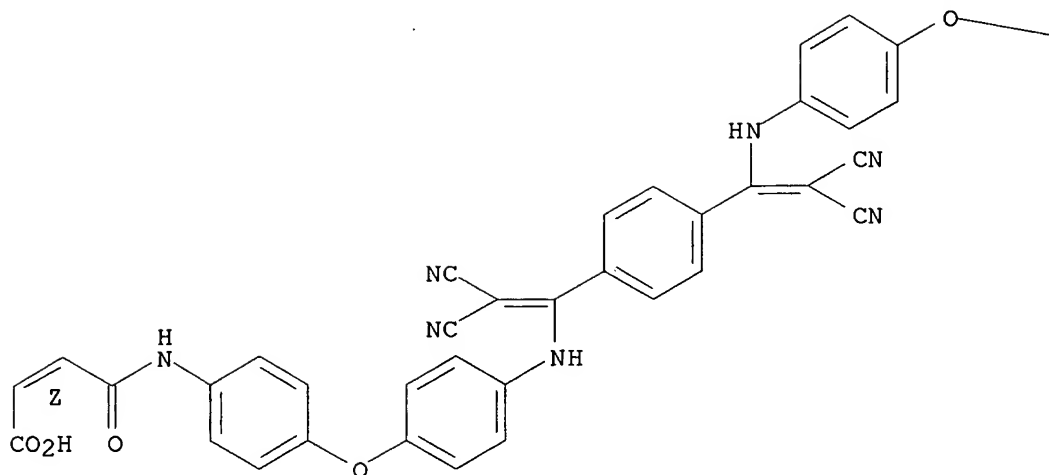
● Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4,4'-[1,4-phenylenebis[(dicyanoethenylidene)imino-4,1-phenyleneoxy-4,1-phenyleneimino]]bis[4-oxo-, (Z,Z)-, homopolymer (9CI)
 MF (C46 H30 N8 O8)x
 CI PMS

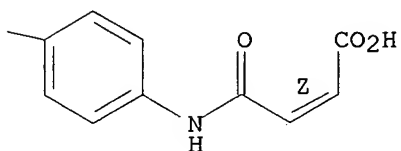
CM 1

Double bond geometry as shown.

PAGE 1-A

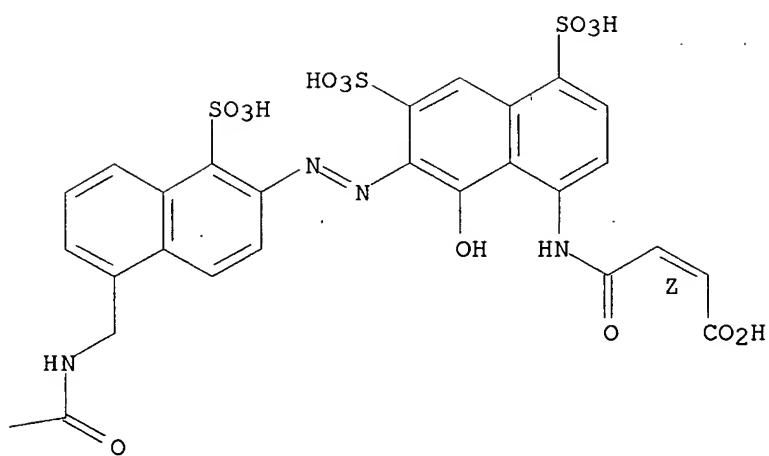
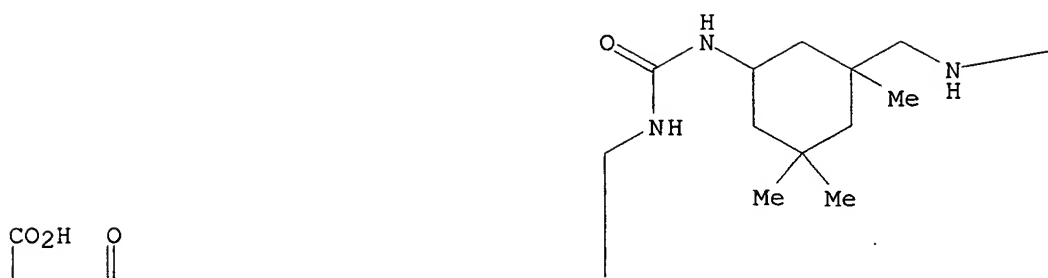


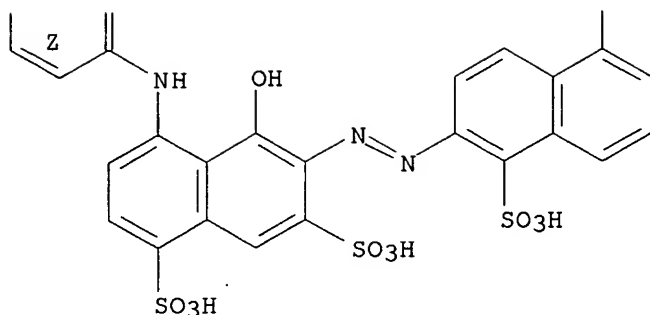
PAGE 1-B



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[[7-[[5-[[[[[3-[[[[[6-[[8-[(3-carboxy-1-oxo-2-propenyl)amino]-1-hydroxy-3,5-disulfo-2-naphthalenyl]azo]-5-sulfo-1-naphthalenyl]methyl]amino]carbonyl]amino]methyl]-3,5,5-trimethylcyclohexyl]amino]carbonyl]amino]methyl]-1-sulfo-2-naphthalenyl]azo]-8-hydroxy-4,6-disulfo-1-naphthalenyl]amino]-4-oxo-, [2Z(2Z)]- (9CI)
 MF C62 H58 N10 O28 S6

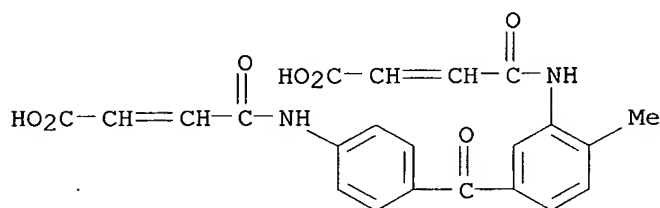
Double bond geometry as described by E or Z.





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

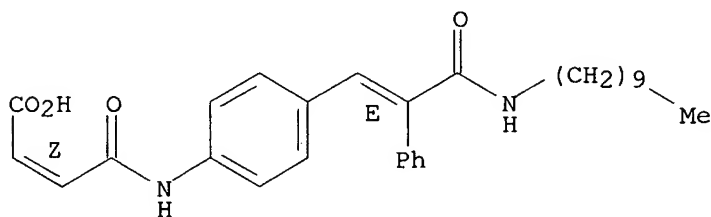
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[[5-[4-[(3-carboxy-1-oxo-2-propenyl)amino]benzoyl]-2-methylphenyl]amino]-4-oxo- (9CI)
 MF C22 H18 N2 O7



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

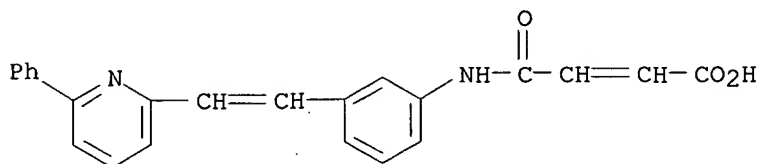
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[[4-[3-(decylamino)-3-oxo-2-phenyl-1-propenyl]phenyl]amino]-4-oxo-, (Z,E)- (9CI)
 MF C29 H36 N2 O4

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

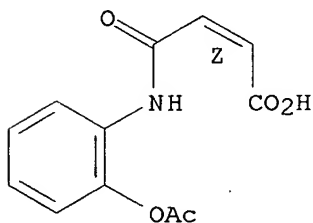
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Butenoic acid,
4-oxo-4-[[3-[2-(6-phenyl-2-pyridinyl)ethenyl]phenyl]amino
]- (9CI)
MF C23 H18 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Maleanilic acid, 2'-hydroxy-, acetate (6CI)
MF C12 H11 N O5

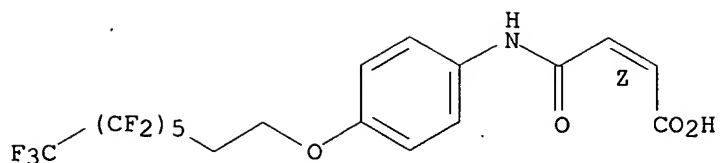
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Butenoic acid, 4-oxo-4-[[4-[(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)oxy]phenyl]amino]-, (Z)- (9CI)
MF C18 H12 F13 N O4

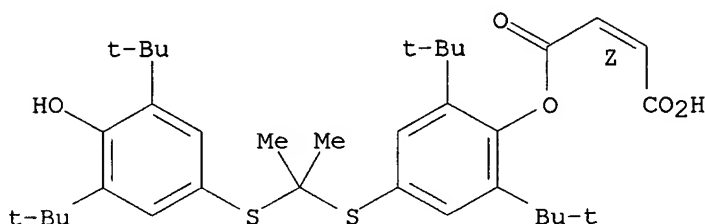
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

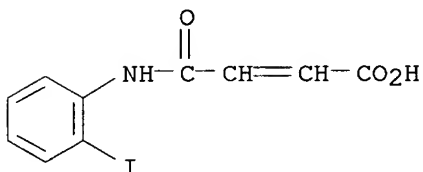
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenedioic acid (2Z)-, mono[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl] ester (9CI)
 MF C35 H50 O5 S2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[(2-iodophenyl)amino]-4-oxo- (9CI)
 MF C10 H8 I N O3

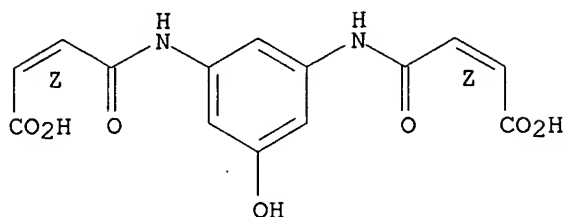


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4,4'-[(5-hydroxy-1,3-phenylene)diimino]bis[4-oxo-, (Z,Z)-

(9CI)
MF C14 H12 N2 O7

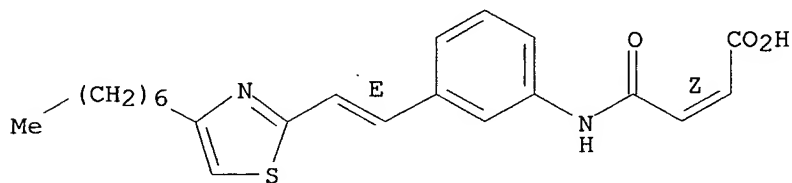
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

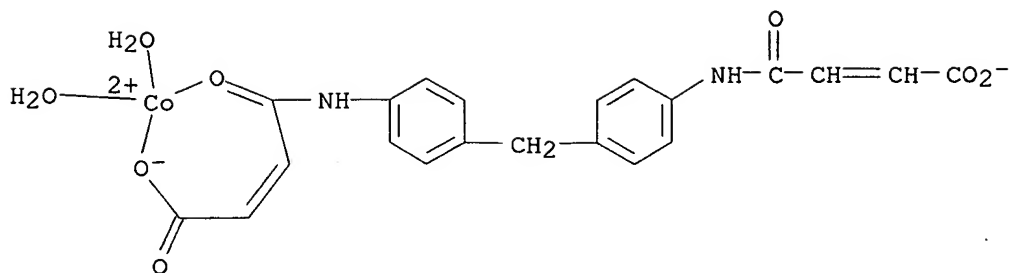
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Butenoic acid, 4-[[3-[2-(4-heptyl-2-thiazolyl)ethenyl]phenyl]amino]-4-oxo-, monosodium salt, (E,Z)- (9CI)
MF C22 H26 N2 O3 S . Na

Double bond geometry as shown.



● Na

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Cobalt, diaqua[[4,4'-[methylenebis(4,1-phenyleneimino)]bis[4-oxo-2-butenato]](2-)-O1,O4]- (9CI)
MF C21 H20 Co N2 O8
CI CCS



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

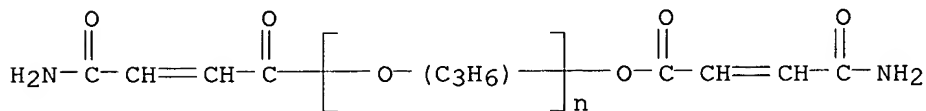
IN 2-Butenoic acid, 4-oxo-4-[(4-sulfophenyl)amino]-, disodium salt, (Z)-, polymer with

(Z,Z)-.alpha.-(4-amino-1,4-dioxo-2-butenyl)-.omega.-[(4-amino-1,4-dioxo-2-butenyl)oxy]poly[oxy(methyl-1,2-ethanediyl)], 2,5-furandione and .alpha.-2-propenyl-.omega.-hydroxypoly(oxy-1,2-ethanediyl) (9CI)

MF (C10 H9 N O6 S . C4 H2 O3 . (C3 H6 O)n C8 H8 N2 O5 . (C2 H4 O)n C3 H6 O . 2 Na)x

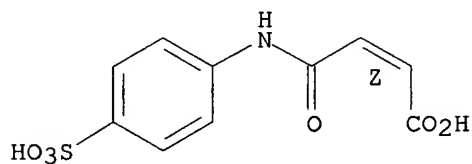
CI PMS, COM

CM 1



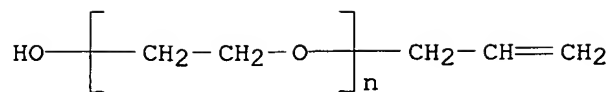
CM 2

Double bond geometry as shown.

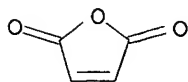


● 2 Na

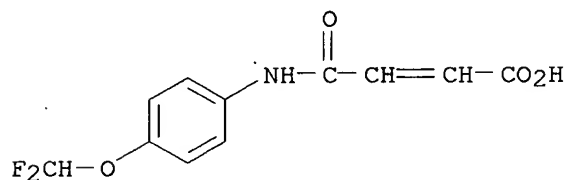
CM 3



CM 4



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 2-Butenoic acid, 4-[[4-(difluoromethoxy)phenyl]amino]-4-oxo- (9CI)
 MF C11 H9 F2 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

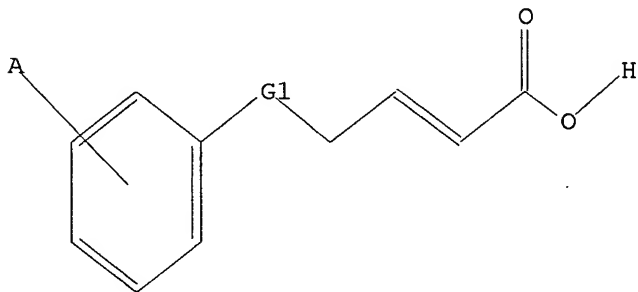
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L3 STRUCTURE UPLOADED

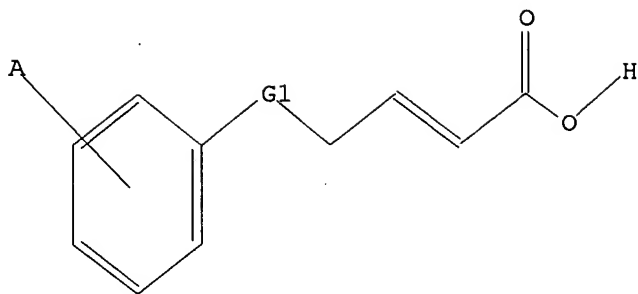
=> d 13

L3 HAS NO ANSWERS

L3 STR



G1 O,S,N



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> search l3 sss sam

SAMPLE SEARCH INITIATED 07:29:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 516 TO ITERATE

100.0% PROCESSED 516 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 8958 TO 11682

PROJECTED ANSWERS: 1 TO 80

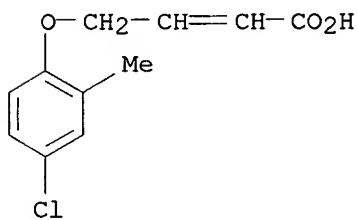
L4 1 SEA SSS SAM L3

=> d scan

L4 1 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 2-Butenoic acid, 4-(4-chloro-2-methylphenoxy)-, ammonium salt (9CI)

MF C11 H11 Cl O3 . H3 N



● NH3

ALL ANSWERS HAVE BEEN SCANNED

=> e 2-Butenoic acid, 4-(4-chloro-2-methylphenoxy)-, ammonium salt/cn

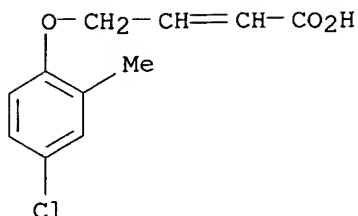
| | | |
|---------|-------|---|
| E1 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, 2-ETHOXYETHYL |
| | | L ESTER/CN |
| E2 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, 2-PROPENYL |
| E | | STER/CN |
| E3 | 1 --> | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, AMMONIUM |
| SAL | | T/CN |
| E4 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, BUTYL |
| ESTER/ | | CN |
| E5 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, COMPD. |
| WITH | | N-METHYLMETHANAMINE (1:1)/CN |
| E6 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, ETHYL |
| ESTER/ | | CN |
| E7 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, METHYL |
| ESTER | | /CN |
| E8 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, PROPYL |
| ESTER | | /CN |
| E9 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, SODIUM |
| SALT/ | | CN |
| E10 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-3-ETHOXY-, |
| ETH | | YL ESTER, (E)-/CN |
| E11 | 1 | 2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENYL)-4-OXO-, |
| (2E)-/C | | N |
| E12 | 1 | 2-BUTENOIC ACID, |
| | | 4-(4-CHLORO-3-METHOXY-5-(METHYLAMINO) PHENYL |
| | |)-3-METHYL-, METHYL ESTER, (E)-/CN |

=> e3

| | | |
|--------|---|---|
| L5 | 1 | "2-BUTENOIC ACID, 4-(4-CHLORO-2-METHYLPHENOXY)-, AMMONIUM |
| SALT"/ | | CN |

=> d 15

| | | | |
|-----|---|-----------------|--------------------|
| L5 | ANSWER 1 OF 1 | REGISTRY | COPYRIGHT 2003 ACS |
| RN | 68838-73-3 | REGISTRY | |
| CN | 2-Butenoic acid, 4-(4-chloro-2-methylphenoxy)-, ammonium salt | | |
| | (9CI) | (CA INDEX NAME) | |
| MF | C11 H11 Cl O3 . H3 N | | |
| LC | STN Files: | CA, CAPLUS | |
| CRN | (68838-71-1) | | |



● NH₃

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

| | | |
|----------------------|------------|---------|
| => file caplus | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 9.90 | 10.11 |

FILE 'CAPLUS' ENTERED AT 07:32:13 ON 12 MAR 2003
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FILE COVERS 1907 - 12 Mar 2003 VOL 138 ISS 11
FILE LAST UPDATED: 11 Mar 2003 (20030311/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l5
l6

1 l5

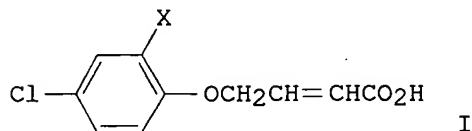
=> d l6 ti fbib abs

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
TI Phenoxyacetonate herbicidal compounds
AN 1979:34995 CAPLUS
DN 90:34995
TI Phenoxyacetonate herbicidal compounds
IN Sadohara, Hideo; Yamauchi, Sanji; Sugiyama, Hidetoshi; Takayama, Shuichi

PA Kumiai Chemical Industry Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|-------------|------|----------|-----------------|----------|
| PI | JP 53101527 | A2 | 19780905 | JP 1977-16837 | 19770217 |
| | | | | JP 1977-16837 | 19770217 |

GI



AB Phenoxyacetonates I (X = Cl or Me) or their alkyl esters, salts, or amides are herbicides. Thus, 4-(2',4'-dichlorophenoxy)crotonic acid [17592-43-7] at 100 g/10 are completely killed Eleocharis acicularia, Cyperus serotinus, Sagittaria pygmaea, Scirpus juncoides, arrowhead, Echinochloa, Monochoria vaginalis, and Cyperus diformia infested in rice fields.

=> logoff hold

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 4.08 | 14.19 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| -0.65 | -0.65 |

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 07:34:46 ON 12 MAR 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal623paz

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web
NEWS 3 Jan 25 Searching with the P indicator for Preparations
NEWS 4 Jan 29 FSTA has been reloaded and moves to weekly updates
NEWS 5 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update
frequency
NEWS 6 Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02
NEWS 7 Mar 08 Gene Names now available in BIOSIS
NEWS 8 Mar 22 TOXLIT no longer available
NEWS 9 Mar 22 TRCTHERMO no longer available
NEWS 10 Mar 28 US Provisional Priorities searched with P in CA/CAPLUS
and USPATFULL
NEWS 11 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY
NEWS 12 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2
instead.
NEWS 13 Apr 08 "Ask CAS" for self-help around the clock

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

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*LBEILSTEIN - BEILSTEIN Learning File

* The files listed above are temporarily unavailable.

FILE 'HOME' ENTERED AT 13:17:15 ON 08 APR 2002

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 13:17:30 ON 08 APR 2002

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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

The P indicator for Preparations was not generated for all of the
CAS Registry Numbers that were added to the H/Z/CA/CAplus files between
12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches
during this period, either directly appended to a CAS Registry Number
or by qualifying an L-number with /P, may have yielded incomplete results.
As of 1/23/02, the situation has been resolved. Also, note that searches
conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files
incorporating CAS Registry Numbers with the P indicator between 12/27/01
and 1/23/02, are encouraged to re-run these strategies. Contact the
CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698,
worldwide, or send an e-mail to help@cas.org for further assistance or to
receive a credit for any duplicate searches.

=>

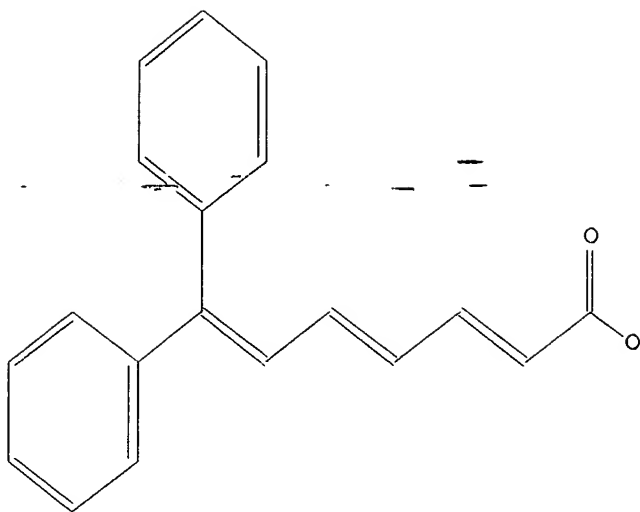
Uploading 10025947 elected specie.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l1 ssssam

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 13:18:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 4 TO 200

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> search l1 sss full

FULL SEARCH INITIATED 13:18:15 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 144 TO ITERATE

100.0% PROCESSED 144 ITERATIONS

2 ANSWERS

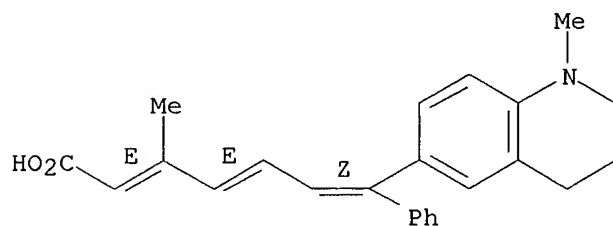
SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> d scan

L3 2 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6-Heptatrienoic acid,
3-methyl-7-phenyl-7-(1,2,3,4-tetrahydro-1-methyl-
6-quinolinyl)-, (2E,4E,6Z)- (9CI)
MF C24 H25 N O2

Double bond geometry as shown.

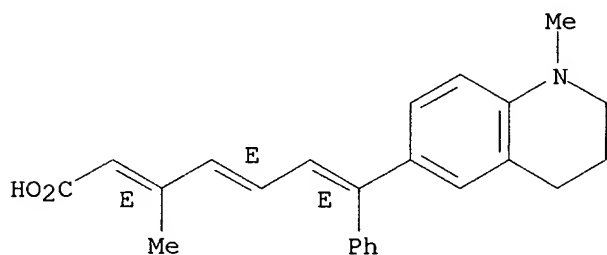


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 2 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6-Heptatrienoic acid,
3-methyl-7-phenyl-7-(1,2,3,4-tetrahydro-1-methyl-
6-quinolinyl)-, (all-E)- (9CI)
MF C24 H25 N O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

ENTRY

141.04

TOTAL

SESSION

141.25

FILE 'CAPLUS' ENTERED AT 13:19:29 ON 08 APR 2002

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FILE COVERS 1907 - 8 Apr 2002 VOL 136 ISS 15
FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 13

L4 1 L3

=> d 14 ti fbib abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

TI Preparation of heterocyclic compounds and mono- or polyenic carboxylic acid derivatives having potent binding activity to retinoid receptors

AN 1996:469506 CAPLUS

DN 125:114703

TI Preparation of heterocyclic compounds and mono- or polyenic carboxylic acid derivatives having potent binding activity to retinoid receptors

IN Hibi, Shigeki; Kikuchi, Kouichi; Yoshimura, Hiroyuki; Nagai, Mitsuo; Tagami, Katsuya; Abe, Shinya; Hishinuma, Ieharu; Nagakawa, Junichi; Miyamoto, Norimasa; et al.

PA Eisai Co., Ltd., Japan

SO PCT Int. Appl., 203 pp.
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 3

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|----------|
| PI | WO 9613478 | A1 | 19960509 | WO 1995-JP2231 | 19951031 |
| | W: AU, CA, CN, FI, HU, KR, MX, NO, NZ, RU, US | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| | JP 1994-267287 A 19941031 | | | | |

| | | | |
|---|----|----------|---------------------------|
| JP 08073464 | A2 | 19960319 | JP 1995-166120 A 19950630 |
| | | | JP 1995-166120 19950630 |
| JP 08208559 | A2 | 19960813 | JP 1994-149795 A 19940630 |
| | | | JP 1995-280165 19951027 |
| AU 9537549 | A1 | 19960523 | JP 1994-267287 A 19941031 |
| | | | AU 1995-37549 19951031 |
| | | | JP 1994-267287 A 19941031 |
| | | | JP 1995-166120 A 19950630 |
| EP 790228 | A1 | 19970820 | WO 1995-JP2231 W 19951031 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IE, IT, LI, LU, NL, PT, SE | | | EP 1995-935597 19951031 |
| | | | JP 1994-267287 A 19941031 |
| | | | JP 1995-166120 A 19950630 |
| US 5977125 | A | 19991102 | WO 1995-JP2231 W 19951031 |
| | | | US 1997-836428 19970506 |
| | | | JP 1994-267287 A 19941031 |
| | | | JP 1995-166120 A 19950630 |
| US 6291508 | B1 | 20010918 | WO 1995-JP2231 W 19951031 |
| | | | US 1999-401732 19990923 |
| | | | JP 1994-267287 A 19941031 |
| | | | JP 1995-166120 A 19950630 |
| | | | WO 1995-JP2231 W 19951031 |
| | | | US 1997-836428 A319970506 |
| | | | US 1998-106112 A319980629 |

PATENT FAMILY INFORMATION:

FAN 1996:367339

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--|----------|----------|---------------------------|----------|
| PI | JP 08073464 | A2 | 19960319 | JP 1995-166120 | 19950630 |
| | | | | JP 1994-149795 A | 19940630 |
| | CA 2202988 | AA | 19960509 | CA 1995-2202988 | 19951031 |
| | | | | JP 1994-267287 A | 19941031 |
| | | | | JP 1995-166120 A | 19950630 |
| | WO 9613478 | A1 | 19960509 | WO 1995-JP2231 | 19951031 |
| | W: AU, CA, CN, FI, HU, KR, MX, NO, NZ, RU, US | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| | | | | JP 1994-267287 A | 19941031 |
| | | | | JP 1995-166120 A | 19950630 |
| AU 9537549 | A1 | 19960523 | | AU 1995-37549 | 19951031 |
| | | | | JP 1994-267287 A | 19941031 |
| | | | | JP 1995-166120 A | 19950630 |
| | | | | WO 1995-JP2231 W | 19951031 |
| EP 790228 | A1 | 19970820 | | EP 1995-935597 | 19951031 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IE, IT, LI, LU, NL, PT, SE | | | | | |
| | | | | JP 1994-267287 A | 19941031 |
| | | | | JP 1995-166120 A | 19950630 |
| | | | | WO 1995-JP2231 W | 19951031 |
| EP 1065203 | A2 | 20010103 | | EP 2000-119709 | 19951031 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE, PT, IE | | | | | |
| | | | | JP 1994-267287 A | 19941031 |
| | | | | JP 1995-166120 A | 19950630 |
| | | | | EP 1995-935597 A319951031 | |
| US 5977125 | A | 19991102 | | US 1997-836428 | 19970506 |
| | | | | JP 1994-267287 A | 19941031 |
| | | | | JP 1995-166120 A | 19950630 |
| | | | | WO 1995-JP2231 W | 19951031 |
| US 6030964 | A | 20000229 | | US 1998-106112 | 19980629 |
| | | | | JP 1994-267287 A | 19941031 |
| | | | | JP 1995-166120 A | 19950630 |

| | | | | |
|------------|----|----------|------------------|----------|
| US 6133283 | A | 20001017 | US 1999-236644 | 19990126 |
| | | | JP 1994-276287 A | 19941031 |
| | | | JP 1995-166120 A | 19950630 |
| US 6291508 | B1 | 20010918 | US 1999-401732 | 19990923 |
| | | | JP 1994-267287 A | 19941031 |
| | | | JP 1995-166120 A | 19950630 |
| | | | WO 1995-JP2231 W | 19951031 |
| | | | US 1997-836428 A | 19970506 |
| | | | US 1998-106112 A | 19980629 |

| | | | | | |
|-----|-------------|------|----------|------------------|----------|
| FAN | 1996:601252 | | | | |
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
| | ----- | --- | ----- | ----- | ----- |
| PI | JP 08188857 | A2 | 19960723 | JP 1995-208140 | 19950815 |
| | | | | JP 1994-276287 A | 19941110 |

OS MARPAT 125:114703

GI For diagram(s), see printed CA Issue.

AB Novel retinoid-related compds. represented by the general formula
Z-(CR3:CR2)nCO2R1 [R1 = H, CO2H-protecting group; R2, R3 = H, halo,

linear

or branched lower alkyl, linear or branched lower alkoxy, aryl; n = 1-3;

n

no. of R2 or R3 are same or different; Z = heterocyclyl such as Q, Q1,

and

Q2; A, B, D = CH, N, S, or S; E = CH, N; F, G = CH, N, S, O; wherein X1, X2, Y1, Y2 = H, NR4R5, CR6R7R8, OR9, S(O)mR10 (m = 0,1,2); wherein R6 - R12 = H, linear or branched alkyl; or X1 and Y2 or X2 and Y2 together

with

the C atoms to which they are bonded form an (un)satd. and

(un)substituted

ring optionally contg. O, S, or N; X3, Y3 = H, linear or branched alkyl

or

alkoxy, cycloalkyl, aryl, heteroaryl, fluoroalkyl, halo; provided that Z .noteq. Ph, 2-naphthyl, etc.) and heterocyclic compds. [I; R1, R2 = H, lower alkyl, alkenylalkyl, alkynylalkyl, cycloalkyl, cycloalkylalkyl, lower alkoxyalkyl, aryl, heteroaryl, arylalkyl; or R1 and R2 together

form

a cycloalkyl ring contg. S, O, SO, SO, NH, or alkylimino; ring A = Q3,

Q4;

wherein R1 and R2 = same as above; Z1 = N, CH; Z2 = O, S, NH, alkylimino; ring B = substituted and unsatd. 5- to 6-membered ring heterocyclyl

contg.

1 or 2 heteroatoms selected from N, O, or S] or physiol. acceptable salts thereof are prepd. These compds. can substitute for retinoic acid as preventives or remedies for various diseases, have potent ability for binding to retinoid receptors (RARs and RXRs), are antagonists of retinoids, and are efficacious in treating various diseases including various keratinization anomalies and rheumatoid arthritis. Thus, (E)-3-(1-isopropyl-1,2,3,4-tetrahydroquinolin-6-yl)-2-butenol (prepn. given) was condensed with 3-methyl-4-phosphonocrotonic acid tri-Et ester in the presence of NaOMe in DMF under ice-cooling for 1 h to give, after sapon., the title compd. (II; R = Q5). II (R = Q6) showed IC50 of 5.4 nM for inhibiting the binding of [3H]-all-trans-retinoic acid to human leukemia HL6-cell fraction and IC50 of 39 nM for antagonizing the all-trans-retinoic acid-induced differentiation of HL6-cells.

=> logoff hold
COST IN U.S. DOLLARS

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |

| | | |
|--|------------|---------|
| FULL ESTIMATED COST | 8.44 | 149.69 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -0.62 | -0.62 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 13:20:10 ON 08 APR 2002

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssstal623paz

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 13:43:47 ON 08 APR 2002
FILE 'CAPLUS' ENTERED AT 13:43:47 ON 08 APR 2002
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| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 8.44 | 149.69 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -0.62 | -0.62 |

=> file reg

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 8.84 | 150.09 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -0.62 | -0.62 |

FILE 'REGISTRY' ENTERED AT 13:44:32 ON 08 APR 2002
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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5
DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover Limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAPLUS files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=>

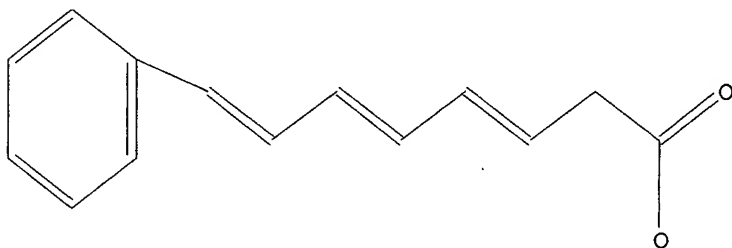
Uploading 10025947 8ph octatrie.str

L5 STRUCTURE UPLOADED

=> d l5

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l5 sss sam

SAMPLE SEARCH INITIATED 13:45:00 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 166 TO ITERATE

100.0% PROCESSED 166 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2547 TO 4093

PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

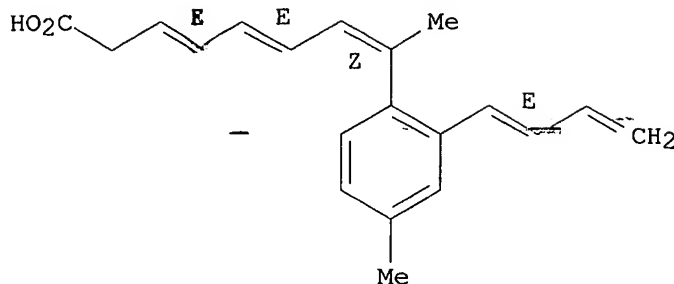
=> d scan

L6 1 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,5,7-Nonatrienoic acid, 8-[2-(1E)-1,3-butadienyl-4-methylphenyl]-, (3E,5E,7Z)- (9CI)

MF C20 H22 O2

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |
| 1.14 | 151.23 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |
| 0.00 | -0.62 |

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 13:46:32 ON 08 APR 2002

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FILE COVERS 007 - 8 Apr 2002 VOL 136 ISS 15

FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your STN profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Rolesthesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the

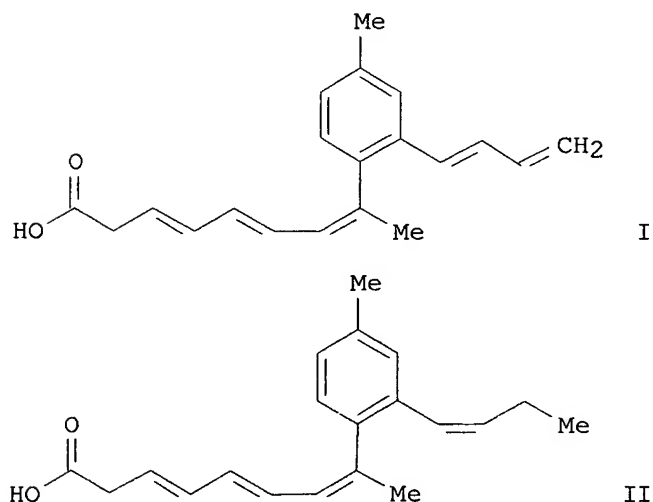
CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 16

L7 1 L6

=> d 17 ti fbib abs

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
TI MF-EA-705.alpha. & MF-EA-705.beta., new metabolites from microbial fermentation of a Streptomyces sp.
AN 2002:11967 CAPLUS
DN 136:213297
TI MF-EA-705.alpha. & MF-EA-705.beta., new metabolites from microbial fermentation of a Streptomyces sp.
AU Qureshi, Asfia; Mauger, Jacob B.; Cano, Raul J.; Galazzo, Jorge L.; Lee, May D.
CS Molecular Diversity and Screening, Microcide Pharmaceuticals, Inc., Mountain View, CA, 94043, USA
SO Journal of Antibiotics (2001), 54(12), 1100-1103
CODEN: JANTAJ; ISSN: 0021-8820
PB Japan Antibiotics Research Association
DT Journal
LA English
GI



AB The prodn., isolation, structure elucidation, and biol. activities of two new compds., MF-EA-705.alpha. (I) and MF-EA-705.beta. (II), were reported.

The prodn. of the bioactive components and their purifn. was monitored by inhibitory activity against Candida albicans in a cut-well agar diffusion assay. MF-EA-705.beta. was isolated as an optically inactive colorless

oil, wherein its mol. formula, C₂₀H₂₄O₂, was 2 amu heavier than that of MF-EA-705.alpha.. The purified compds. MF-EA-705.alpha. and MF-EA-705.beta. were inactive at a concn. of 128 .mu.g/mL against Candida albicans, C. glabrata, C. krusei, Cryptococcus neoformans, and

Aspergillus

fumigatus. The min. inhibitory concn. (MIC) of MF-EA-705.alpha. against C. albicans was 1 mg/mL, indicating the unsuitability of this compd. as a drug candidate. The activity noted and followed during bioassay-guided fractionation was thus because of high concns. of the compd. being

assayed

in the cut-well agar plates. Nevertheless, these compds. are novel metabolites, with a comparable compd. having been isolated only once previously in the microbial natural product literature.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff hold

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 3.08 | 154.31 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | -0.62 | -1.24 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 13:47:27 ON 08 APR 2002

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal623paz

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 13:49:27 ON 08 APR 2002
FILE 'CAPLUS' ENTERED AT 13:49:27 ON 08 APR 2002
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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 3.08 | 154.31 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | -0.62 | -1.24 |

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 3.08 | 154.31 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | -0.62 | -1.24 |

FILE 'REGISTRY' ENTERED AT 13:49:34 ON 08 APR 2002
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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5
DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TECA INFORMATION NOW CURRENT THROUGH July 7, 2001

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Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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or by qualifying an L-number with /P, may have yielded incomplete results.
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incorporating CAS Registry Numbers with the P indicator between 12/27/01
and 1/23/02, are encouraged to re-run these strategies. Contact the
CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698,
worldwide, or send an e-mail to help@cas.org for further assistance or to
receive a credit for any duplicate searches.

⇒ file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.38 | 154.69 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CAS SUBSCRIBER PRICE | 0.00 | -1.24 |

FILE 'REGISTRY' ENTERED AT 13:49:45 ON 08 APR 2002
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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5
DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TECA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> e 4-phenylbutanoic acid/cn

| | | |
|-----|-------|---|
| E1 | 1 | 4-PHENYLBUTANOATE/CN |
| E2 | 1 | 4-PHENYLBUTANOATE ION(1-)/CN |
| E3 | 1 --> | 4-PHENYLBUTANOIC ACID/CN |
| E4 | 1 | 4-PHENYLBUTANOIC ACID COMPD. WITH DIBENZO-18-CROWN-6/CN |
| E5 | 1 | 4-PHENYLBUTANOL/CN |
| E6 | 1 | 4-PHENYLBUTANOLIDE/CN |
| E7 | 1 | 4-PHENYLBUTANOYL CHLORIDE/CN |
| E8 | 1 | 4-PHENYLBUTANOYLFERROCENE/CN |
| E9 | 1 | 4-PHENYLBUTENONE/CN |
| E10 | 1 | 4-PHENYLBUTYL/CN |
| E11 | 1 | 4-PHENYLBUTYL (4-PHENYLBUTYL) CARBAMATE/CN |
| E12 | 1 | 4-PHENYLBUTYL 5-AMINO-4-OXOPENTANOATE HYDROCHLORIDE/CN |

=> e3

L8 1 "4-PHENYLBUTANOIC ACID"/CN

=> d 18

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 1821-12-1 REGISTRY
CN Benzenebutanoic acid (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Butyric acid, 4-phenyl- (8CI)
OTHER NAMES:
CN .gamma.-Phenylbutanoic acid
CN .gamma.-Phenylbutyric acid
CN .omega.-Phenylbutanoic acid
CN 4-Phenyl-n-butyric acid
CN **4-Phenylbutanoic acid**
CN 4-Phenylbutyric acid
CN Benzenebutyric acid
FS 3D CONCORD
MF C10 H12 O2
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DDFU,

DRUGU, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, SPECINFO,
 SYNTHLINE, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)

HO₂C—(CH₂)₃—Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

577 REFERENCES IN FILE CA (1967 TO DATE)
 13 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 579 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 5.96 | 160.65 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.24 |

FILE 'CAPLUS' ENTERED AT 13:50:27 ON 08 APR 2002
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FILE COVERS 1907 - 8 Apr 2002 VOL 136 ISS 15
 FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/Caplus files incorporating CAS Registry

Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 18

L9 582 L8

=> 18/prep

582 L8
2849417 PREP/RL
L10 45 L8/PREP
(L8 (L) PREP/RL)

=> d 110 45 ti fbib abs

L10 ANSWER 45 OF 45 CAPLUS COPYRIGHT 2002 ACS

TI Dismutation of 3,4-dihydronaphthalenic compounds. II.

AN 1967:421719 CAPLUS

DN 67:21719

TI Dismutation of 3,4-dihydronaphthalenic compounds. II.

AU Quillet, Jean P.; Duperrier, A.; Dreux, Jacques

CS Ecole Super. Chim. Ind., Lyon, Fr.

SO Bull. Soc. Chim. Fr. (1967), (1), 255-60

CODEN: BSCFAS

DT Journal

LA French

GI For diagram(s), see printed CA Issue.

AB cf. CA 64: 14122c. Ketones of the type I were treated with MeMgI to give II. The dismutation of II (R = R1 = R2 = H) gave a mixt. contg. 1-methyl-1,2,3,4-tetrahydronaphthalene (III) and 1-MeC10H7 (IV). Thus, a mixt. of 93 g. PhCH2CH2CH(CO2Et)2 and 800 ml. 5% NaOH was refluxed 3 hrs. to give 90% 4-phenylbutyric acid (V), b15 170-1.degree.. Also prepd.

were

PhCHR2CHR1CHRCO2H (R, R1, R2, b.p./mm., m.p., and % yield given): Me, H, H, -, -, -; H, H, Ph, 185-9.degree./1, 103-6.degree., 70; H, Ph, H, 188-9.degree./0.3, 92-3.degree., 70; Ph, H, H, -, 70-1.degree., 70. V (1 mole) was treated with 150 g. SOCl2 to give 4-phenylbutyryl chloride

(VI).

Similarly prepd. were PhCHR2CHR1CHRCOCl (R, R1, and R2 given): Me, H, H; H, H, Ph; H, Ph, H; Ph, H, H. VI (70 g.) was treated with 51 g. AlCl3 in C6H6 and the mixt. hydrolyzed with HCl to give 70% 1-tetralone (VII), b12 129-30.degree.. Similarly prepd. were I (R, R1, R2, b.p./mm., m.p., and

%

yield given): H, Me, H, 133-4.degree./13, -, 74 (semicarbazone m. 189.degree.); Me, H, H, -, -, -; H, H, Ph, 135-40.degree./0.1,

76.degree.,

81; H, Ph, H, 162-5.degree./0.1, 64.degree., 81; Ph, H, H, 170.degree./0.3, 76.degree., 79. A soln. of 22 g. VII in ether was treated with a soln. contg. MeMgI (prepd. from 23.5 g. MeI and 3.6 g. Mg) to give 57% 1-methyl-1-tetralol, m. 86.degree., which was dehydrated to give 1-methyl-3,4-dihydronaphthalene (VIII). Similarly prepd. were II

(R,

R1, R2, b.p./mm., n25D, and % yield given): H, Me, H, 116.degree./18, 1.559, 58; Me, H, H, -, -, -; H, H, Ph, 130-2.degree./1, -, 80; H, Ph, H, 132-5.degree./2.5, 1.611, 60; Ph, H, H, -, -, 72 (m. 76.degree.). VII (1 g.) was added dropwise to 7 ml. H2SO4 to give a mixt. contg. 3% VII, 54% III, and 43% IV. A mixt. of 1 g. VIII in 10 ml. HBr azeotrope was refluxed 1 hr. to give a mixt. of 64% VIII, 19% III, and 17% IV. A mixt. of 1 g. VIII and 10 ml. Bradsher reagent (CA 40: 57069) was refluxed 30 min. to give a mixt. contg. 16% VIII, 41.5% III, and 42.5% IV as compared

with 6.5, 51, and 42, resp., after 1.5 hrs. of refluxing. The other II, when treated with Bradsher reagent, behaved similarly.

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

5.10

165.75

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.62

-1.86

FILE 'REGISTRY' ENTERED AT 13:52:17 ON 08 APR 2002

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DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> e 5-phenylpentanoic acid/cn

E1 1 5-PHENYLPENTANETHIOL/CN

E2 1 5-PHENYLPENTANOATE ION(1-)/CN

E3 1--> 5-PHENYLPENTANOIC ACID/CN

E4 1 5-PHENYLPENTANOIC ACID

(2-(4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZO

L-4-YL)ETHYL)AMIDE MONO(TRIFLUOROACETATE)/CN

E5 1 5-PHENYLPENTANOIC ACID

(4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZOL-4

-YLMETHYL)AMIDE MONO(TRIFLUOROACETATE)/CN

E6 1 5-PHENYLPENTANOIC ACID

(4,5,6,7-TETRAHYDRO-1H-BENZIMIDAZOL-5

-YL)AMIDE HYDROCHLORIDE/CN
 E7 1 5-PHENYLPENTANOIC PERACID/CN
 E8 1 5-PHENYLPENTANOL/CN
 E9 1 5-PHENYLPENTANOYL CHLORIDE/CN
 E10 1 5-PHENYLPENTANOYLFERROCENE/CN
 E11 1 5-PHENYLPENTYL BROMIDE/CN
 E12 1 5-PHENYLPENTYL CHLORIDE/CN

=> e3

L11 1 "5-PHENYLPENTANOIC ACID"/CN

=> d l11

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN 2270-20-4 REGISTRY
 CN Benzenepentanoic acid (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Valeric acid, 5-phenyl- (6CI, 7CI, 8CI)
 OTHER NAMES:
 CN .delta.-Phenylvaleric acid
 CN **5-Phenylpentanoic acid**
 CN 5-Phenylvaleric acid
 CN Phenylpentanoic acid
 CN Phenylvaleric acid
 FS 3D CONCORD
 MF C11 H14 O2
 CI COM
 LC STN Files: AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA,
 CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHM,
 EMBASE, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, RTECS*, SPECINFO,
 TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**
 (**Enter CHEMLIST File for up-to-date regulatory information)

HO₂C-(CH₂)₄-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

268 REFERENCES IN FILE CA (1967 TO DATE)
 5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 268 REFERENCES IN FILE CAPLUS (1967 TO DATE)
 22 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

| | | |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 6.34 | 172.09 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.86 |

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FILE COVERS 1907 - 8 Apr 2002 VOL 136 ISS 15
FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> l11

L12 269 L11

=> l11/prep

269 L11
2849417 PREP/RL
L13 28 L11/PREP
(L11 (L) PREP/RL)

=> d l13 28 ti fbib abs

L13 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2002 ACS
TI Fermentation process for preparing cinnamic acid and 5-phenylvaleric acid
AN 1967:84752 CAPLUS
DN 66:84752
TI Fermentation process for preparing cinnamic acid and 5-phenylvaleric acid
IN Douros, John D., Jr.; Frankenfeld, John W.
PA Esso Research and Engineering Co.
SO U.S., 5 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|----------|
| | ----- | ---- | ----- | ----- | ----- |
| PI | US 3301766 | | 19670131 | US | 19640923 |
| AB | Cinnamic acid (I) and 5-phenylvaleric acid (II) are prepd. by the | | | | |

fermentation of n-alkylated benzenes contg. an odd (3-15) no. of C-atoms in the n-alkyl side chain, using Pseudomonas ligustri, P. pseudomallei,

P.

orvilla, Alcaligenes, Cellulomonas galba, and Brevibacterium healii ATCC 15522-15527. The microorganism is fermented for 18-26 hrs. in a growth medium before adding the alkylated benzene. II can be harvested selectively for the 1st 18 hrs. of fermentation, and I for the next

20-144

hrs. In an example, 100 ml. of a sterile growth medium contg. n-hexadecane 2, K₂HPO₄ 0.5, (NH₄)₂HPO₄ 1, Na₂SO₄ 0.05, MgSO₄·7H₂O 0.04, FeSO₄·7H₂O 0.002, MnSO₄·4H₂O 0.002, and NaCl 0.002% (wt.) was inoculated with C. galba ATCC 15526 previously cultured for 24 hrs. at 30.degree. in the same medium. n-Amylbenzene (0.35 g.) was added and fermentation continued for 96 hrs., with shaking. There was complete conversion of

the

benzene to I (91%) and II (9%).

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

9.06

181.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.62

-2.48

FILE 'REGISTRY' ENTERED AT 14:01:18 ON 08 APR 2002

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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698,

worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> e cinammoylhydroxamic acid/cn

| | | |
|-----|-------|---|
| E1 | 1 | CINAMETIC ACID/CN |
| E2 | 1 | CINAMIODYL/CN |
| E3 | 0 --> | CINAMMOYLHYDROXAMIC ACID/CN |
| E4 | 1 | CINAMMYLAMINE, N,N,.BETA.-TRIMETHYL-/CN |
| E5 | 1 | CINAMODIOL/CN |
| E6 | 1 | CINAMOLOL/CN |
| E7 | 1 | CINANSERIN/CN |
| E8 | 1 | CINANSERIN HYDROCHLORIDE/CN |
| E9 | 1 | CINANSERINE/CN |
| E10 | 1 | CINAPROXEN/CN |
| E11 | 1 | CINARCAF/CN |
| E12 | 1 | CINARIN/CN |

=> e cinammoylhydroxamic acid/cn

| | | |
|-----|-------|---|
| E1 | 1 | CINAMIODYL/CN |
| E2 | 1 | CINAMMYLAMINE, N,N,.BETA.-TRIMETHYL-/CN |
| E3 | 0 --> | CINAMMYLHYDROXAMIC ACID/CN |
| E4 | 1 | CINAMODIOL/CN |
| E5 | 1 | CINAMOLOL/CN |
| E6 | 1 | CINANSERIN/CN |
| E7 | 1 | CINANSERIN HYDROCHLORIDE/CN |
| E8 | 1 | CINANSERINE/CN |
| E9 | 1 | CINAPROXEN/CN |
| E10 | 1 | CINARCAF/CN |
| E11 | 1 | CINARIN/CN |
| E12 | 1 | CINARIOLIDE/CN |

=> save temp all deactylase/l

L# LIST 1-L13 HAS BEEN SAVED AS 'DEACTYLASE/L'

=> logoff hold

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 1.90 | 183.05 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | 0.00 | -2.48 |

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 14:04:07 ON 08 APR 2002

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Welcome to STN International! Enter x:x

LOGINID:ssptal623paz

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
 NEWS 2 Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web
 NEWS 3 Jan 25 Searching with the P indicator for Preparations
 NEWS 4 Jan 29 FSTA has been reloaded and moves to weekly updates
 NEWS 5 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency
 NEWS 6 Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02
 NEWS 7 Mar 08 Gene Names now available in BIOSIS
 NEWS 8 Mar 22 TOXLIT no longer available
 NEWS 9 Mar 22 TRCTHERMO no longer available
 NEWS 10 Mar 28 US Provisional Priorities searched with P in CA/CAplus and USPATFULL
 NEWS 11 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY
 NEWS 12 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead.
 NEWS 13 Apr 08 "Ask CAS" for self-help around the clock

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002

NEWS HOURS STN Operating Hours Plus Help Desk Availability
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 NEWS WWW CAS World Wide Web Site (general information)

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* * * * * STN Columbus * * * * *

*LBEILSTEIN - BEILSTEIN Learning File

* The files listed above are temporarily unavailable.

FILE 'DME' ENTERED AT 06:39:07 ON 09 APR 2002

=> file reg

| | | |
|----------------------|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 06:39:19 ON 09 APR 2002
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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/ST/STNOTES/stnotes27.pdf>

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Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=>

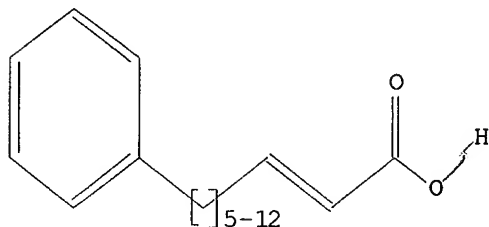
Uploading 10025947 2nd try.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 06:40:38 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 584 TO ITERATE

100.0% PROCESSED 584 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

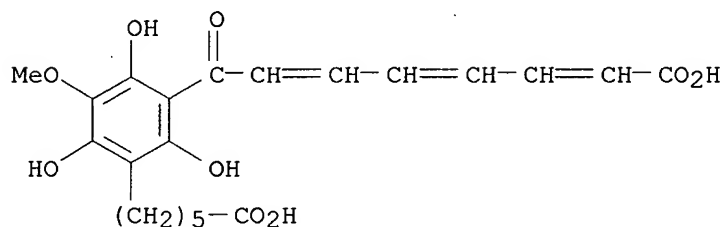
FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
PROJECTED ITERATIONS: 10231 TO 13129
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d scan

L2 1 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenehexanoic acid, 3-(7-carboxy-1-oxo-2,4,6-heptatrienyl)-2,4,6-
trihydroxy-5-methoxy- (9CI)
MF C21 H24 O9



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l1 sss full

FULL SEARCH INITIATED 06:41:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11383 TO ITERATE

100.0% PROCESSED 11383 ITERATIONS
SEARCH TIME: 00.00.03

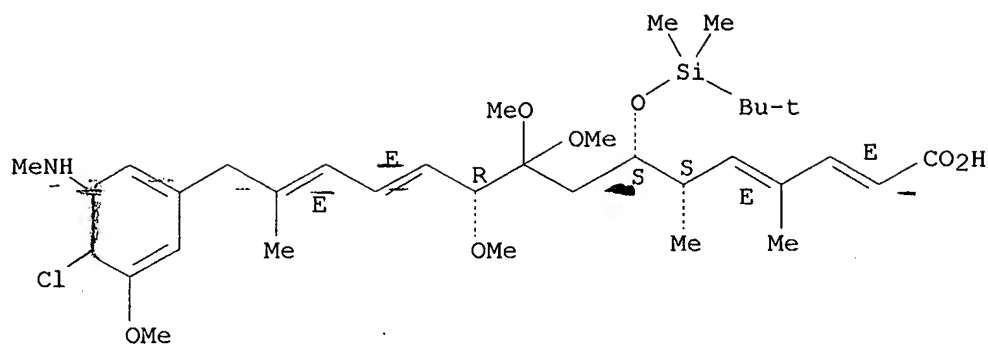
64 ANSWERS

L3 64 SEA SSS FUL L1

=> d scan

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,11,13-Pentadecatetraenoic acid, 15-[4-chloro-3-methoxy-5-
(methylamino)phenyl]-7-[[1,1-dimethylethyl)dimethylsilyl]oxy]-9,9,10-
trimethoxy-4,6,14-trimethyl-, (2E,4E,6R*,7R*,10S*,11E,13E)- (9CI)
MF C35 H56 Cl N O7 Si

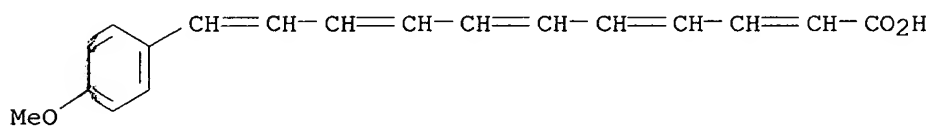
Relative stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

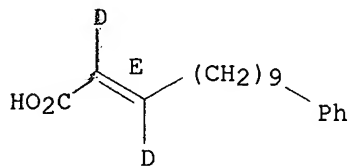
L3 4 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 14,6,8,10-Undecapentaenoic acid, 11-(p-methoxyphenyl)- (6CI)
 MF C18 H18 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 4 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Dodecenoic-2,3-d2 acid, 12-phenyl-, sodium salt, (E)- (9CI)
 MF C18 H24 D2 O2 . Na

Double bond geometry as shown.

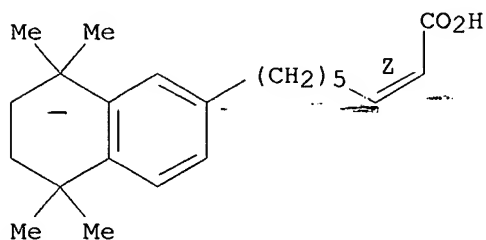


● Na

L3 4 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Octenoic acid,
 8-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-
 , (Z)- (9CI)

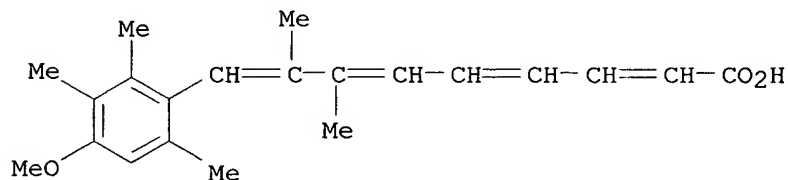
MF C22 H32 O2

Double bond geometry as shown.



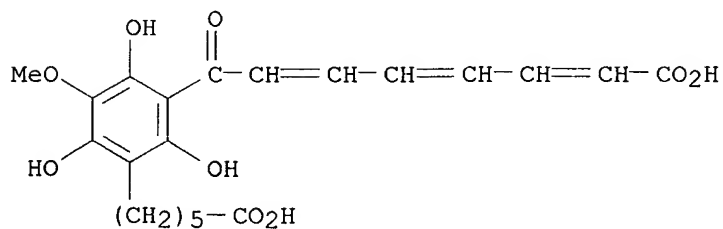
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6,8-Nonatetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)-7,8-dimethyl- (9CI)
MF C21 H26 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenehexanoic acid, 3-(7-carboxy-1-oxo-2,4,6-heptatrienyl)-2,4,6-trihydroxy-5-methoxy- (9CI)
MF C21 H24 O9



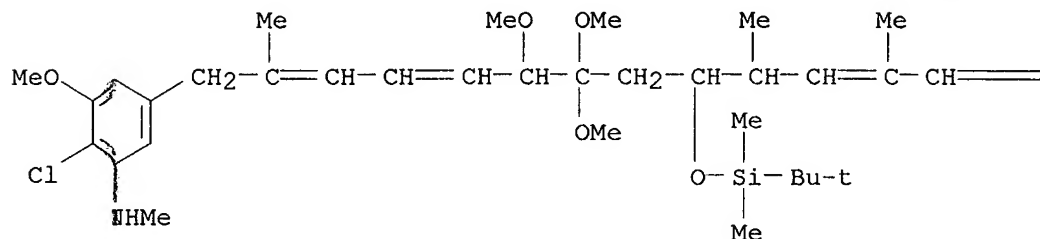
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-titanaminium, N,N,N-tributyl-, salt with
 (2E,4E,6E,7R*,10S*,11E,13E)-15-
 [4-chloro-3-methoxy-5-(methylamino)phenyl]-7-[[[(1,1-
 dimethylethyl)dimethylsilyl]oxy]-9,9,10-trimethoxy-4,6,14-trimethyl-
 2,4,11,13-pentadecatetraenoic acid (1:1) (9CI)
 MF C31 H55 Cl N O7 Si . C16 H36 N

CM 1

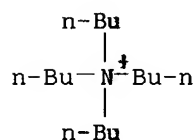
PAGE 1-A



PAGE 1-B

=CH-CO⁻

CM 2

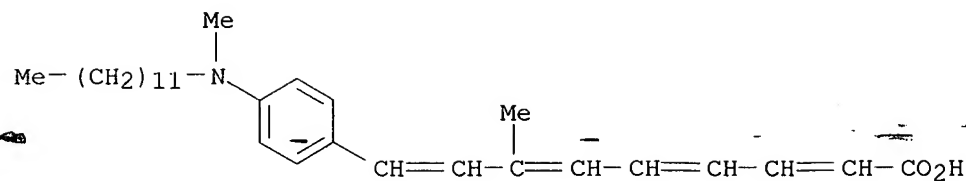


L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8-Nonatetraenoic acid, 9-phenyl- (9CI)
 MF C15 H14 O2

Ph-CH=CH-CH=CH-CH=CH-CH=CH-CO₂H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

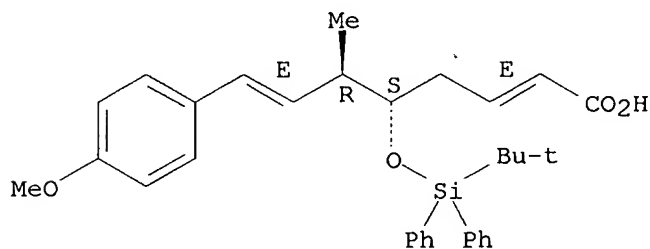
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8-Nonatetraenoic acid, 9-[4-(dodecylmethylamino)phenyl]-7-methyl-
 (9CI)
 MF C29 H43 N O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,7-Octadienoic acid, 5-[[[1,1-dimethylethyl)diphenylsilyl]oxy]-8-(4-methoxyphenyl)-6-methyl-, [S-[R*,S*-(E,E)]]- (9CI)
 MF C32 H38 O4 Si

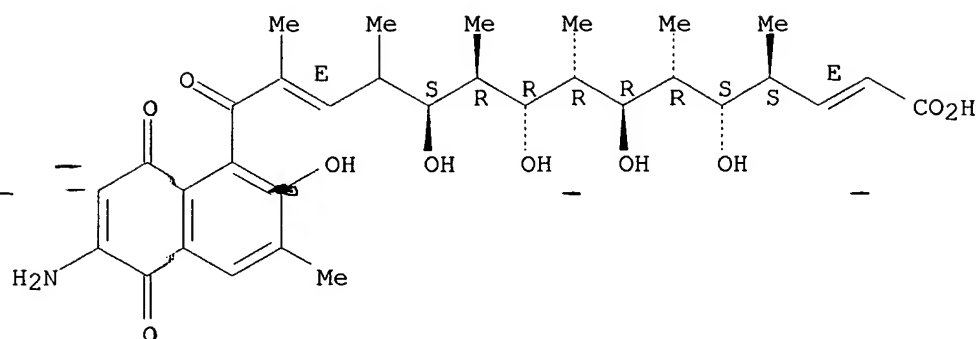
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,13-Pentadecadienoic acid,
 15-[(6-amino-5,8-dihydro-2-hydroxy-3-methyl-5,8-dioxo-1-naphthalenyl)-5,7,9,11-tetrahydroxy-4,6,8,10,12,14-hexamethyl-15-oxo-, (2E,4S,5S,6R,7R,8R,9R,10R,11S,13E)]- (9CI)
 MF C32 H43 N O10

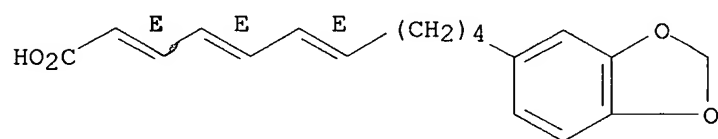
Absolute stereochemistry.
 Double bond geometry as shown.
 Currently available stereo shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

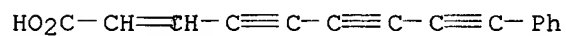
L3 64 ~~ANSWERS~~ REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6-Undecatetraenoic acid, 11-(1,3-benzodioxol-5-yl)-, (E,E,E,E)- (9CI)
 MF C18 ~~H2~~ O4

Double bond geometry as shown.



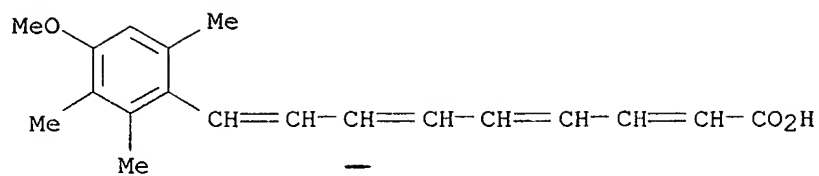
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ~~ANSWERS~~ REGISTRY COPYRIGHT 2002 ACS
 IN 2-Nonene-4,6,8-triynoic acid, 9-phenyl- (6CI, 7CI)
 MF C15 ~~H2~~ O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

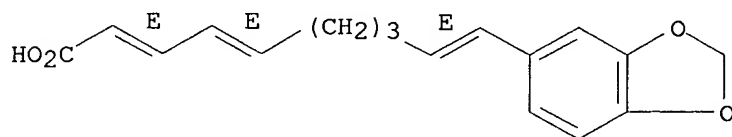
L3 64 ~~ANSWERS~~ REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8-Nonatetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)- (9CI)
 MF C19 ~~H2~~ O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,9-Decatrienoic acid, 10-(1,3-benzodioxol-5-yl)-, (E,E,E)- (9CI)
 MF C17 H18 O4

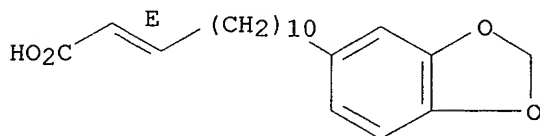
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Tridecenoic acid, 13-(1,3-benzodioxol-5-yl)-, (E)- (9CI)
 MF C20 H28 O4

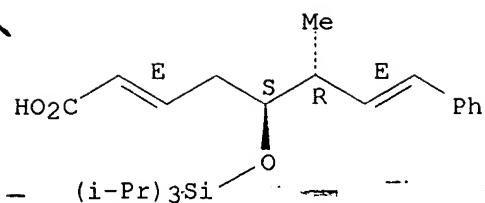
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,7-Octadienoic acid,
 6-methyl-8-phenyl-5-[[tris(1-methylethyl)silyl]oxy]-
 , (2E,5S,6R,7E)- (9CI)
 MF C24 H38 O3 Si

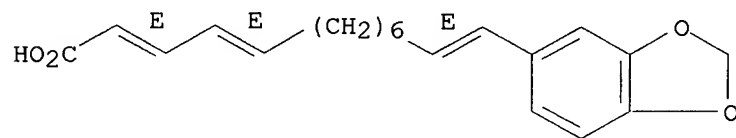
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

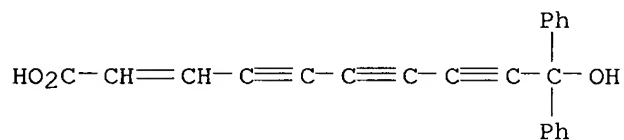
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,12-Tridecatrienoic acid, 13-(1,3-benzodioxol-5-yl)-, (E,E,E)- (9CI)
 MF C20 H24 O4

Double bond geometry as shown.



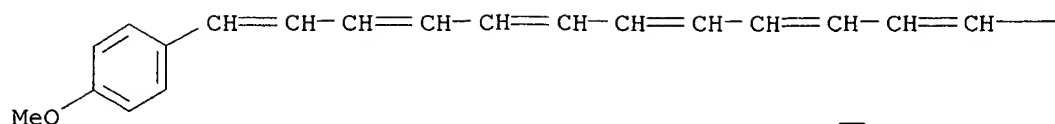
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Decene-4,6,8-triynoic acid, 10-hydroxy-10,10-diphenyl- (6CI, 7CI)
 MF C22 H14 O3

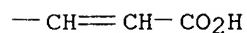


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8,10,12,14-Pentadecaheptaenoic acid, 15-(p-methoxyphenyl)-,
 potassium salt (6CI)
 MF C22 H22 O3 . K

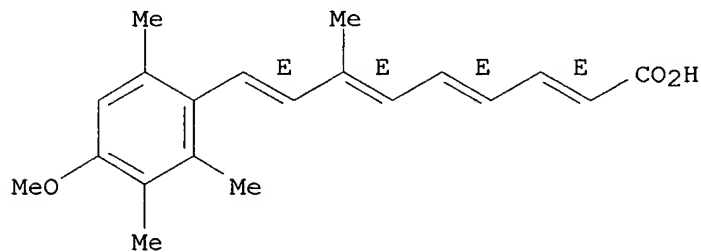


● K



L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8-Nonatetraenoic acid,
 9-(4-methoxy-2,3,6-trimethylphenyl)-7-methyl-
 , (all-E)- (9CI)
 MF C20 H24 O3

Double bond geometry as shown.

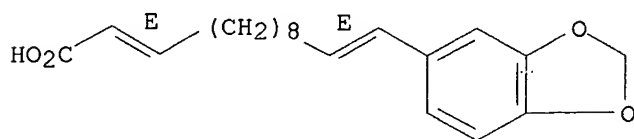


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,12-Tridecadienoic acid, 13-(1,3-benzodioxol-5-yl)-, (E,E)- (9CI)
 MF C20 H26 O4

Double bond geometry as shown.

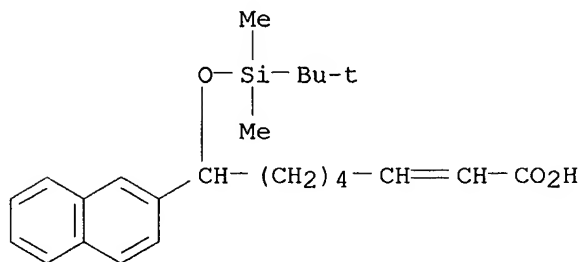


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Octenoic acid, 8-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-(2-naphthalenyl)- (9CI)

MF C24 H34 O3 Si



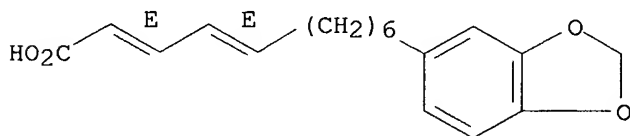
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4-Undecadienoic acid, 11-(1,3-benzodioxol-5-yl)-, (2E,4E)- (9CI)

MF C18 H22 O4

Double bond geometry as shown.



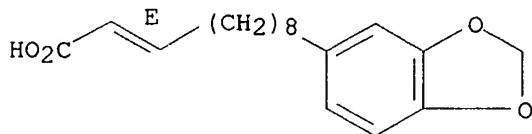
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Undecenoic acid, 11-(1,3-benzodioxol-5-yl)-, (E)- (9CI)

MF C18 H24 O4

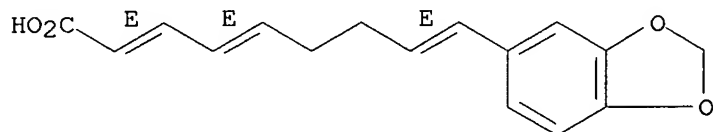
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,8-Nonatrienoic acid, 9-(1,3-benzodioxol-5-yl)-, (E,E,E)- (9CI)
MF C16 H16 O4

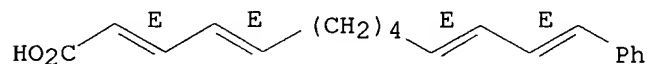
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,10,12-Tridecatetraenoic acid, 13-phenyl-, (all-E)- (9CI)
MF C19 H22 O2

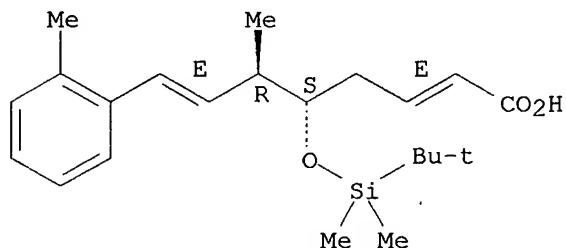
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,7-Octadienoic acid,
5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-8-(
2-methylphenyl)-, [S-[R*,S*-(E,E)]]- (9CI)
MF C22 H34 O3 Si

Absolute stereochemistry.
Double bond geometry as shown.

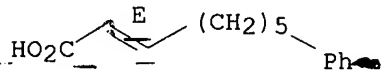


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Octenoic acid, 8-phenyl-, (2E)- (9CI)
MF C~~14~~ H18 O2

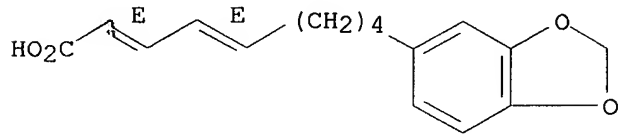
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4-Nonadienoic acid, 9-(1,3-benzodioxol-5-yl)-, (E,E)- (9CI)
MF C~~15~~ H18 O4

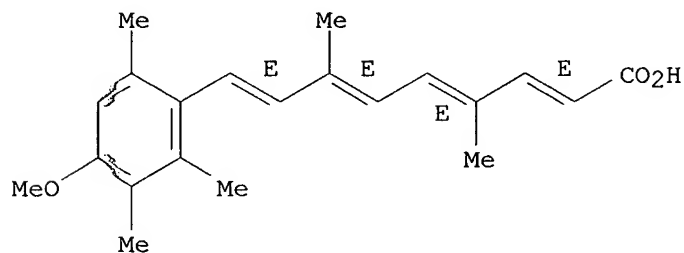
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6,8-Nonatetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)-4,7-dimethyl-, (all-E)- (9CI)
MF C~~21~~ H26 O3

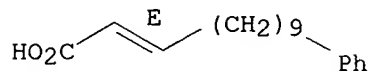
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

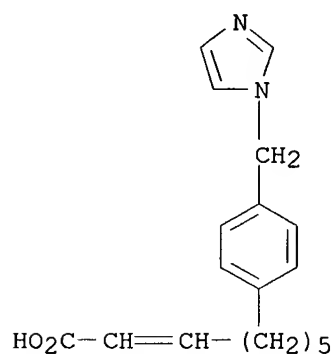
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2-Dodecenoic acid, 12-phenyl-, (E)- (9CI)
MF C~~17~~ H26 O2
CI C~~17~~

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

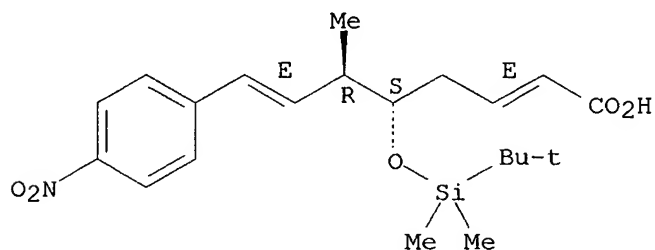
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2-Octenoic acid, 8-[4-(1H-imidazol-1-ylmethyl)phenyl]- (9CI)
MF C18 H22 N2 O2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

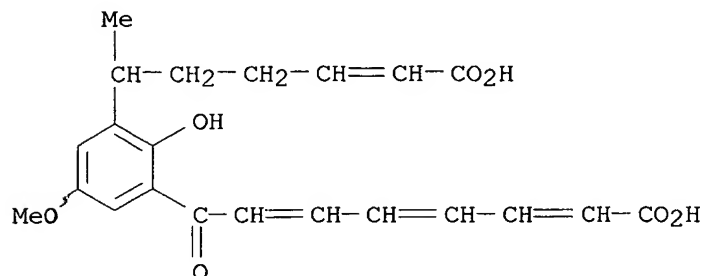
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,7-Octadienoic acid,
5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-8-(
4-nitrophenyl)-, [S-[R*,S*-(E,E)]]- (9CI)
MF C21 H31 N O5 Si

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

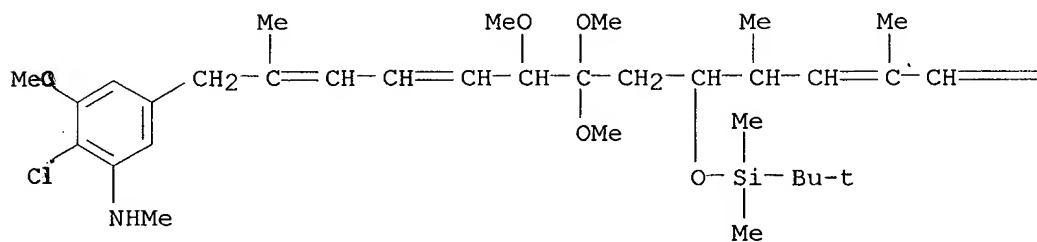
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6-Octatrienoic acid,
 8-[3-(5-carboxy-1-methyl-4-pentenyl)-2-hydroxy-5-
 methoxyphenyl]-8-oxo- (9CI)
 MF C22 H24 O7



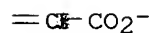
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,11,13-Pentadecatetraenoic acid, 15-[4-chloro-3-methoxy-5-
 (methylamino)phenyl]-7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-9,9,10-
 trimethoxy-4,16,14-trimethyl-, ion(1-), (2E,4E,6R*,7R*,10S*,11E,13E)-
 (9CI)
 MF C35 H55 Cl N O7 Si
 CI COM

PAGE 1-A

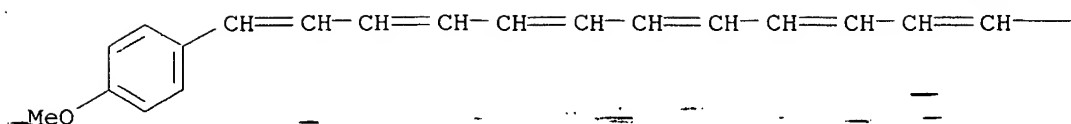


PAGE 1-B

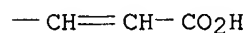


L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8,10,12,14-Pentadecaheptaenoic acid, 15-(p-methoxyphenyl)- (6CI)
 MF C22 H22 O3
 CI COM

PAGE 1-A



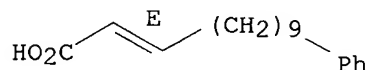
PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2-Dodecenoic acid, 12-phenyl-, sodium salt, (E)- (9CI)
MF C18 H26 O2 . Na

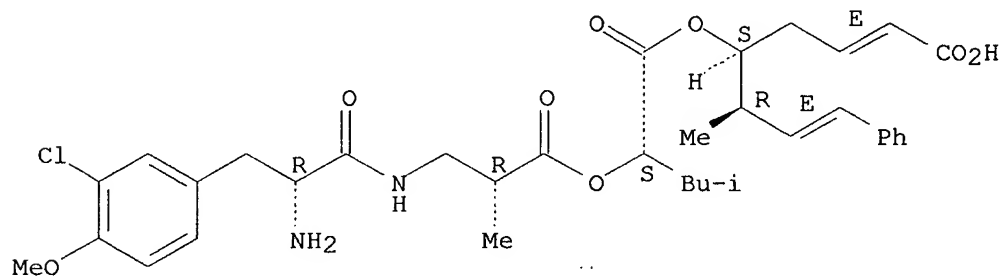
Double bond geometry as shown.



● Na

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Pentanoic acid,
3-chloro-O-methyl-D-tyrosyl-(2R)-2-methyl-.beta.-alanyl-2-
hydroxy-4-methyl-, (1S,2R,3E)-1-[(2E)-3-carboxy-2-propenyl]-2-methyl-4-
phenyl-3-butenyl ester, (2S)- (9CI)
MF C35 H45 Cl N2 O8

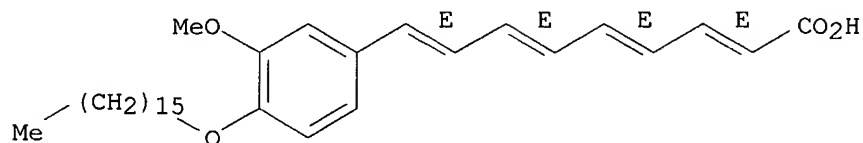
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6,8-Nonatetraenoic acid, 9-[4-(hexadecyloxy)-3-methoxyphenyl]-,
(2E,4E,6E,8E)- (9CI)
MF C32 H48 O4

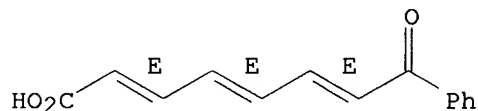
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4,6-Octatrienoic acid, 8-oxo-8-phenyl-, (E,E,E)- (9CI)
MF C14 H12 O3

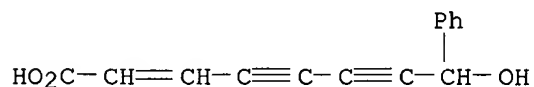
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):25

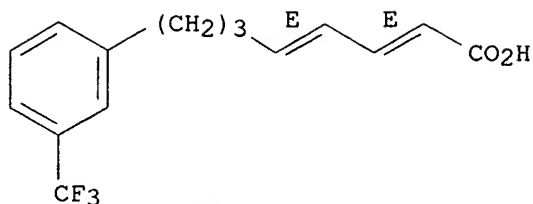
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2-Octene-4,6-diynoic acid, 8-hydroxy-8-phenyl- (7CI)
MF C14 H10 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2,4-Octadienoic acid, 8-[3-(trifluoromethyl)phenyl]-, (E,E)- (9CI)
MF C15 H15 F3 O2

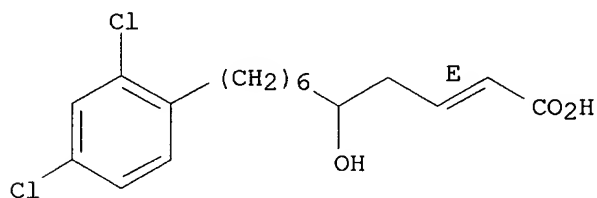
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Undecenoic acid, 11-(2,4-dichlorophenyl)-5-hydroxy-, (E)- (9CI)
 MF C17 H22 Cl2 O3

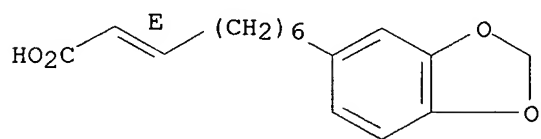
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Nonenoic acid, 9-(1,3-benzodioxol-5-yl)-, (E)- (9CI)
 MF C16 H20 O4

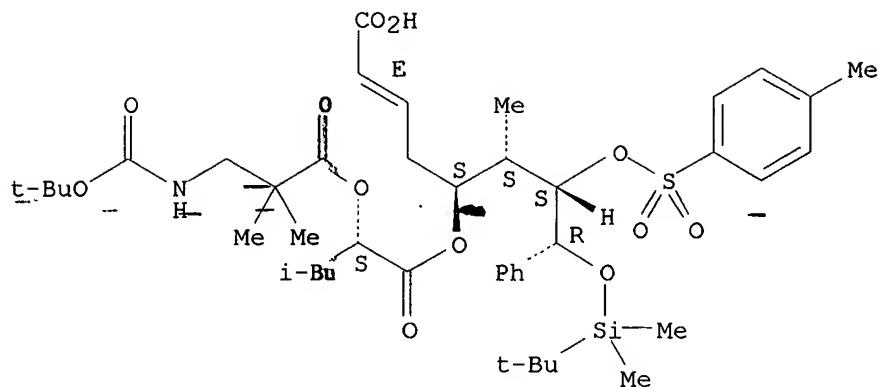
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 6,9,14-Trioxa-2-aza-15-silaheptadecanoic acid, 10-[(2E)-3-carboxy-2-propenyl]-4,4,11,15,15,16,16-heptamethyl-12-[[4-methylphenyl)sulfonyl]oxy]-7-(2-methylpropyl)-5,8-dioxo-13-phenyl-, 1-(1,1-dimethylethyl) ester, (7S,10S,11S,12S,13R)- (9CI)
 MF C44 H67 N O12 S Si

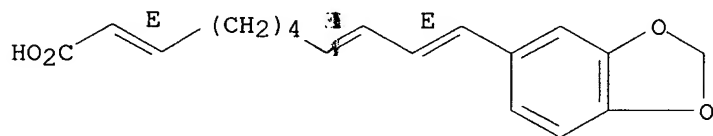
Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

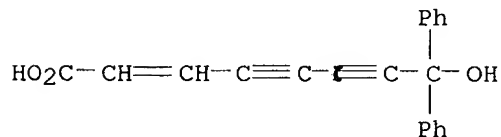
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,8,10-Undecatrienoic acid, 11-(1,3-benzodioxol-5-yl)-, (E,E,E)- (9CI)
 MF C18 H20 O4

Double bond geometry as shown.



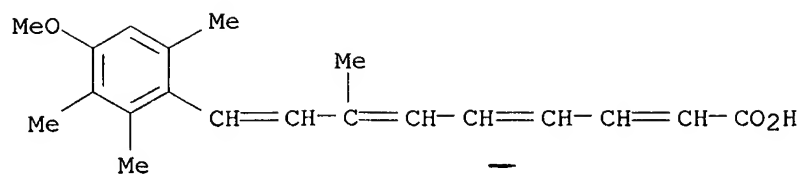
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Octene-4,6-dienoic acid, 8-hydroxy-8,8-diphenyl- (6CI, 7CI)
 MF C20 H14 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

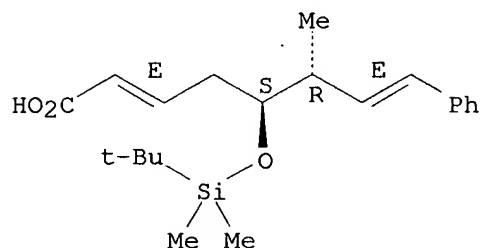
L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8-Nonatetraenoic acid,
 9-(4-methoxy-2,3,6-trimethylphenyl)-7-methyl-
 (9CI)
 MF C20 H24 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,7-Octadienoic acid,
 5-[[1,1-dimethylethyl)dimethylsilyl]oxy]-6-methyl-8-
 phenyl-, (2E,5S,6R,7E)- (9CI)
 MF C21 H32 O3 Si

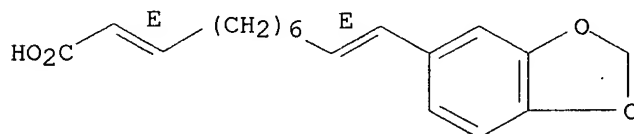
Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,10-Undecadienoic acid, 11-(1,3-benzodioxol-5-yl)-, (E,E)- (9CI)
 MF C18 H22 O4

Double bond geometry as shown.



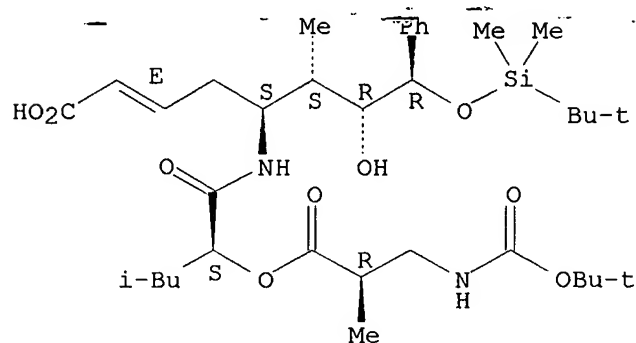
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 6,14-Dioxa-2,9-diaza-15-silaheptadecanoic acid, 10-[(2E)-3-carboxy-2-
 propenyl]-12-hydroxy-4,11,15,15,16,16-hexamethyl-7-(2-methylpropyl)-5,8-
 phenyl-, (2E,5S,6R,7E)- (9CI)

dioxo-13-phenyl-, 1-(1,1-dimethylethyl) ester, (4R,7S,10S,11S,12R,13R)-
(9CI)

MF C36 H60 N2 O9 Si

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



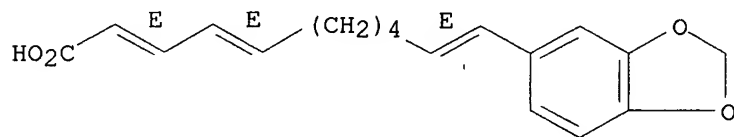
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,4,10-Undecatrienoic acid, 11-(1,3-benzodioxol-5-yl)-, (2E,4E,10E)-
(9CI)

MF C18 H20 O4

Double bond geometry as shown.



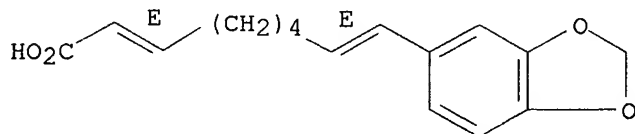
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,8-Nonadienoic acid, 9-(1,3-benzodioxol-5-yl)-, (E,E)- (9CI)

MF C16 H18 O4

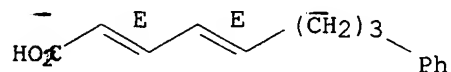
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4-Octadienoic acid, 8-phenyl-, (E,E)- (9CI)
 MF C14 H16 O2

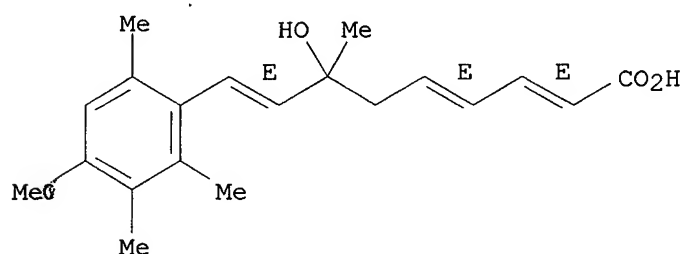
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,8-Nonatrienoic acid, 7-hydroxy-9-(4-methoxy-2,3,6-trimethylphenyl)-7-methyl-, (E,E,E)- (9CI)
 MF C20 H26 O4

Double bond geometry as shown.

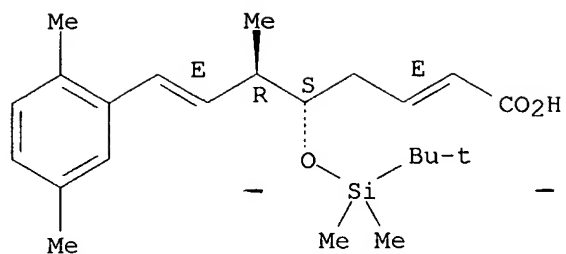


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,7-Octadienoic acid, 5-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-(2,5-dimethylphenyl)-6-methyl-, [S-[R*,S*-(E,E)]]- (9CI)
 MF C23 H36 O3 Si

Absolute stereochemistry.

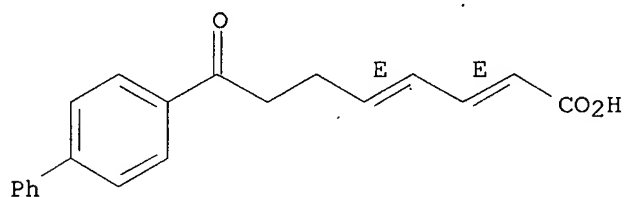
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4-Octadienoic acid, 8-[1,1'-biphenyl]-4-yl-8-oxo-, (2E,4E)- (9CI)
 MF C20 H18 O3

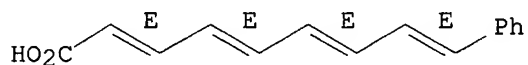
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8-Nonatetraenoic acid, 9-phenyl-, (all-E)- (9CI)
 MF C15 H14 O2

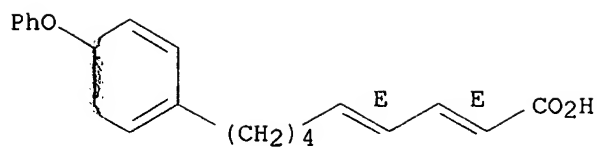
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4-Nonadienoic acid, 9-(4-phenoxyphenyl)-, (E,E)- (9CI)
 MF C21 H22 O3

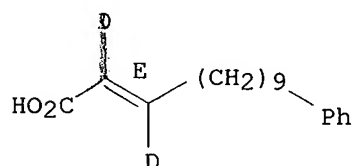
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

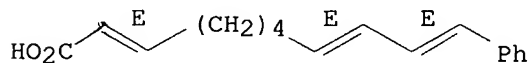
L3 ~~4~~ ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2-Dodecenoic-2,3-d2 acid, 12-phenyl-, (E)- (9CI)
 MF ~~18~~ H24 D2 O2
 CI ~~2M~~

Doublebond geometry as shown.



L3 ~~6~~ ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,8,10-Undecatrienoic acid, 11-phenyl-, (all-E)- (9CI)
 MF ~~17~~ H20 O2

Doublebond geometry as shown.

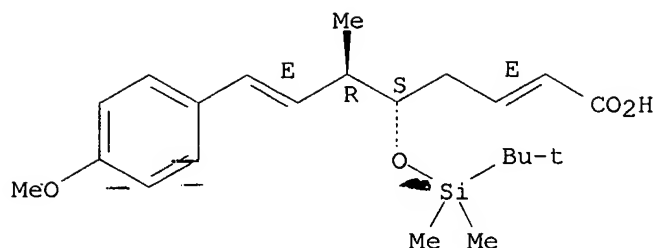


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 ~~6~~ ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,7-Octadienoic acid, 5-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-8-(4-methoxyphenyl)-6-methyl-, [S-[R*,S*-(E,E)]]- (9CI)
 MF ~~12~~ H34 O4 Si

Absolute stereochemistry.

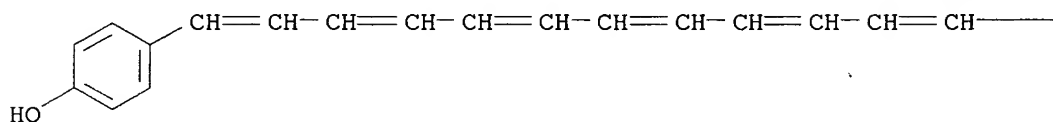
Doublebond geometry as shown.



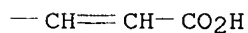
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 64 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 2,4,6,8,10,12,14-Pentadecaheptaenoic acid, 15-(4-hydroxyphenyl)- (9CI)
 MF C21 H20 O3

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

144.08

144.29

FILE 'CAPLUS' ENTERED AT 06:46:02 ON 09 APR 2002

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FILE COVERS 1907 - 9 Apr 2002 VOL 136 ISS 15
FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Bles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SHs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 13

L4 65 L3

=> save temp alkylenes/a
ENTER L#, L# RANGE, ALL, OR (END):14
ANSWER ~~SW~~ L4 HAS BEEN SAVED AS 'ALKYLENES/A'

=> file eg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.40 | 144.69 |

FILE 'REGISTRY' ENTERED AT 06:46:47 ON 09 APR 2002
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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5
DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry file, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAPLUS files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results.

As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> e 2-Dodecenoic acid, 12-phenyl-/cn

E1 1 2-DODECENOIC ACID, 12-OXO-, METHYL ESTER, (E)-/CN
E2 1 2-DODECENOIC ACID, 12-OXO-2-((TRIMETHYLSILYL)METHYL)-, ETHYL ESTER, (Z)-/CN
E3 0 --> 2-DODECENOIC ACID, 12-PHENYL-/CN
E4 1 2-DODECENOIC ACID, 12-PHENYL-, (E)-/CN
E5 1 2-DODECENOIC ACID, 12-PHENYL-, SODIUM SALT, (E)-/CN
E6 1 2-DODECENOIC ACID, 2,3,7,11-TETRAMETHYL-, ETHYL ESTER/CN
E7 1 2-DODECENOIC ACID, 2,4,7,11-TETRAMETHYL-, METHYL ESTER/CN
E8 1 2-DODECENOIC ACID, 2,7,11-TRIMETHYL-6-(1-METHYLETHENYL)-, ETHYL ESTER, (R*,R*-(E))-/CN
E9 1 2-DODECENOIC ACID, 2,7,11-TRIMETHYL-6-(1-METHYLETHENYL)-, ETHYL ESTER, (R*,R*-(Z))-/CN
E10 1 2-DODECENOIC ACID, 2-(((2,2-DIMETHYLCYCLOPROPYL)CARBONYL)AMINO)-, (Z)-/CN
E11 1 2-DODECENOIC ACID, 2-(((2,2-DIMETHYLCYCLOPROPYL)CARBONYL)AMINO)-, (Z)-(.+.-)/CN
E12 1 2-DODECENOIC ACID, 2-((1-OXOPENTYL)OXY)-, ETHYL ESTER/CN

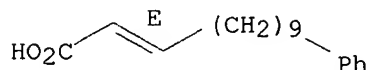
=> e4

L5 1 "2-DODECENOIC ACID, 12-PHENYL-, (E)-"/CN

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 127251-32-5 REGISTRY
CN 2-Dodecenoic acid, 12-phenyl-, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H26 O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

6.34

151.03

FILE 'CAPLUS' ENTERED AT 06:47:59 ON 09 APR 2002

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FILE COVERS 1907 - 9 Apr 2002 VOL 136 ISS 15

FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 15

L6 3 L5

=> d 16 1-3 ti fbib abs

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS

TI Evaluation of the steric course of enoyl reduction in higher plants and insects via coupling to 1-alkene biosynthesis. A model study with *Parthamus tinctorius* (Asteraceae) and *Tribolium castaneum* (Coleoptera; Tenebrionidae)

AN 1992:125172 CAPLUS

DN 16:125172

TI Evaluation of the steric course of enoyl reduction in higher plants and insects via coupling to 1-alkene biosynthesis. A model study with *Parthamus tinctorius* (Asteraceae) and *Tribolium castaneum* (Coleoptera; Tenebrionidae)

AU Froessl, Christian; Boland, Wilhelm

CS Inst. Opt. Chem., Univ. Karlsruhe, Karlsruhe, D-7500/1, Germany
SO J. Chem. Soc., Chem. Commun. (1991), (24), 1731-3
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
AB (E)-12-Phenyl[2-2H₂]dodec-2-enoic acid is in vivo reduced and oxidatively decarboxylated by plant (*Carthamus tinctorius*) and insect (*Tribolium castaneum*) model systems to (Z)-11-phenyl[1-2H]undec-1-ene. The known anti-elimination of the carboxy group and the C(3)-H_s hydrogen atom in conjunction with the (Z)-configuration of the alkene demands an anti-2Re,3Re addn. of two hydrogen atoms across the double bond of the precursor acid.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS

TI Additional enoates and other .alpha.,.beta.-unsaturated carbonyl compounds

as substrates for the enoate reductase from *Clostridium tyrobutyricum*, influence of elevated hydrogen pressure on the reduction rate

AN 1990:511414 CAPLUS

DN 113:111414

TI Additional enoates and other .alpha.,.beta.-unsaturated carbonyl compounds

as substrates for the enoate reductase from *Clostridium tyrobutyricum*, influence of elevated hydrogen pressure on the reduction rate

AU Preiss, U.; White, H.; Simon, H.

CS Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.

SO DECHEMA Biotechnol. Conf. (1989), 3(Pt. A, Jt. Meet. SIM DECHEMA, Presentation Biochem. Lab., Microb. Princ. Bioprocesses, Appl. Genet.), 189-92

CODEN: DBCOEU

DT Journal

LA English

AB Enoates with a soly. of only 30 .mu.M can be hydrogenated on a preparative

scale (280 mmol/3 ltr). For vols. >300 mL and for substrates, which are rapidly reduced by enoate reductase, it is advantageous to carry out the hydrogenations at elevated H pressure. Conditions were found by which cells of *C. tyrobutyricum* can be freeze-dried without any loss of activity. These cells are stable for several months in the absence of O₂. Freeze dried cells were used for the stereospecific deuteration of different enoates. The C-C double bonds of various hitherto unstudied substrates and .beta.,.gamma.-unsatd. .alpha.-keto acids were reduced by enoate reductase.

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS

TI Synthesis of chiral 12-phenyl(2H)dodecanoic acids: useful metabolic probes for the biosynthesis of 1-alkenes from fatty acids

AN 1990:235013 CAPLUS

DN 112:235013

TI Synthesis of chiral 12-phenyl(2H)dodecanoic acids: useful metabolic probes for the biosynthesis of 1-alkenes from fatty acids

AU Goergen, Guenther; Boland, Wilhelm; Preiss, Ute; Simon, Helmut

CS Inst. Org. Chem., Karlsruhe, D-7500, Fed. Rep. Ger.

SO Helv. Chim. Acta (1989), 72(5), 917-28

CODEN: HCACAV; ISSN: 0018-019X

DT Journal

LA English

OS CASREACT 112:235013

AB Chiral 12-phenyl(2H)dodecanoic acids were prepd. as metabolic probes for

the evaluation of the stereochem. course of the biosynthesis of 1-alkenes from fatty acids in plants and insects. The (2R,3R)- or (2S,3S)-Ph(CH₂)₉(CHD)2CO₂H are obtained in high chem. and optical yield (>97% e.e.) from (E)-Ph(CH₂)₉CD:CDCO₂H or (E)-Ph(CH₂)₉CH:CHCO₂H by redn. with Clostridium tyrobutyricum in either 2H₂O or H₂O buffer. The (2R)- and (2S)-Ph(CH₂)₁₀CHDCO₂H are accessible from (E)-Ph(CH₂)₁₀CD:CDCH₂OH via Sharpless epoxidn. The (E)- and (Z)-Ph(CH₂)₉CH:CHD were prep'd. as ref. compds.

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

8.85

159.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.86

-1.86

FILE 'REGISTRY' ENTERED AT 06:51:12 ON 09 APR 2002

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STRUCTURE FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

DICTIONARY FILE UPDATES: 7 APR 2002 HIGHEST RN 404565-89-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAPLUS files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> e 2,4-Octadienoic acid, 8-phenyl-/CN

E1 1 2,4-OCTADIENOIC ACID, 8-OXO-, METHYL ESTER, (E,E)-/CN

E2 1 2,4-OCTADIENOIC ACID, 8-OXO-8-(PHENYLAMINO)-, METHYL ESTER,

(2E,4E)-/CN

E3 0 --> 2,4-OCTADIENOIC ACID, 8-PHENYL-/CN
 E4 1 2,4-OCTADIENOIC ACID, 8-PHENYL-, (E,E)-/CN
 E5 1 2,4-OCTADIENOIC ACID, 8-PHENYL-, ETHYL ESTER, (E,E)-/CN
 E6 1 2,4-OCTADIENOIC ACID,
 9A-(ACETYLOXY)-1A,1B,4,4A,5,7A,7B,8,9,

9A-DECAHYDRO-4A,7B-DIHYDROXY-3-(HYDROXYMETHYL)-1,1,6,8-TETRA
 METHYL-5-OXO-1H-CYCLOPROPA(3,4) BENZ(1,2-E) AZULEN-9-YL
 ESTER,

(1AR-(1A.ALPHA.,1B./CN
 E7 2 2,4-OCTADIENOIC ACID,
 9A-(ACETYLOXY)-1A,1B,4,4A,5,7A,7B,8,9,

9A-DECAHYDRO-7B-HYDROXY-3-(HYDROXYMETHYL)-1,1,6,8-TETRAMETHY
 L-5-OXO-1H-CYCLOPROPA(3,4) BENZ(1,2-E) AZULEN-9-YL ESTER,
 (1AR

-(1A.ALPHA.,1B.BETA./CN
 E8 1 2,4-OCTADIENOIC ACID,
 9A-(ACETYLOXY)-3-(ACETYLOXY)METHYL)-1

A,1B,4,4A,5,7A,7B,8,9,9A-DECAHYDRO-4A,7B-DIHYDROXY-1,1,6,8-T
 ETAMETHYL-5-OXO-1H-CYCLOPROPA(3,4) BENZ(1,2-E) AZULEN-9-YL
 ES

TER, (1AR-(1A.ALPHA./CN
 E9 1 2,4-OCTADIENOIC ACID,
 9A-(ACETYLOXY)-3-(ACETYLOXY)METHYL)-1

A,1B,4,4A,5,7A,7B,8,9,9A-DECAHYDRO-7B-HYDROXY-1,1,6,8-TETRAM
 ETHYL-5-OXO-1H-CYCLOPROPA(3,4) BENZ(1,2-E) AZULEN-9-YL
 ESTER,

(1AR-(1A.ALPHA.,1B.B/CN
 E10 1 2,4-OCTADIENOIC ACID,
 9A-(ACETYLOXY)-3-(ACETYLOXY)METHYL)-1

A,1B,4,4A,5,7A,7B,8,9,9A-DECAHYDRO-7B-HYDROXY-1,1,6-TRIMETHY
 L-5-OXO-1H-CYCLOPROPA(3,4) BENZ(1,2-E) AZULEN-9-YL ESTER,
 (1A.

ALPHA.,1B.BETA.,4A.B/CN
 E11 1 2,4-OCTADIENOIC ACID, ANHYDRIDE WITH ACETIC ACID, (E,E)-/CN
 E12 1 2,4-OCTADIENOIC ACID, ETHYL ESTER/CN

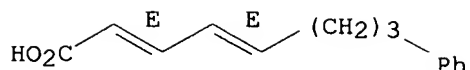
=> e4

L7 1 "2,4-OCTADIENOIC ACID, 8-PHENYL-, (E,E)-"/CN

=> d 17

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
 RN 111985-62-7 REGISTRY
 CN 2,4-Octadienoic acid, 8-phenyl-, (E,E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C14 H16 O2
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> file caplus

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 5.96 | 165.84 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 0.00 | -1.86 |

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FILE COVERS 1907 - 9 Apr 2002 VOL 136 ISS 15
FILE LAST UPDATED: 7 Apr 2002 (20020407/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> 17

L8

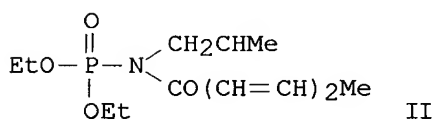
1 L7

=> d 18 ti fbib abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
TI Preparation of alkenamides and thioalkenamides as pesticides
AN 1988:21522 CAPLUS
DN 108:21522
TI Preparation of alkenamides and thioalkenamides as pesticides
IN Black, Malcolm Henry; Blade, Robert John; Peek, Robert John
PA Wellcome Foundation Ltd., UK
SO Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|----------|
| PI | EP 228853 | A2 | 19870715 | EP 1986-309741 | 19861215 |
| | EP 228853 | A3 | 19890315 | | |
| | EP 228853 | B1 | 19920722 | | |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | | | | GB 1985-31072 | 19851217 |
| | US 5037813 | A | 19910806 | US 1986-940561 | 19861211 |
| | | | | GB 1985-31072 | 19851217 |
| | JP 62187442 | A2 | 19870815 | JP 1986-298593 | 19861215 |
| | | | | GB 1985-31072 | 19851217 |
| | AT 78461 | E | 19920815 | AT 1986-309741 | 19861215 |
| | | | | GB 1985-31072 | 19851217 |
| | | | | EP 1986-309741 | 19861215 |
| | ES 2042503 | T3 | 19931216 | ES 1986-309741 | 19861215 |
| | | | | GB 1985-31072 | 19851217 |
| | US 5091414 | A | 19920225 | US 1990-619872 | 19901129 |
| | | | | US 1986-940561 | 19861211 |
| | US 5124348 | A | 19920623 | US 1991-701834 | 19910517 |
| | | | | GB 1985-31072 | 19851217 |
| | | | | US 1986-940561 | 19861211 |

GI



AB Title compds. R1(AC:CA1)nCC(:X)NR2R3 [I; R1 = (substituted)alkyl; R2 = (substituted)alkyl, (substituted)alkenyl; (substituted)cycloalkyl; R3 = Y(:X1)(R4)a, S(O)bR5, S(O)bNR6R7, NR2C(:X)(AlC:CA)R1; A,Al = H, alkyl, haloalkyl; X, X1 = O, S; Y = P, C; R4 = H, alkyl, alkoxy, acyl, alkoxy carbonyl; R5 = alkyl, aryl, aryloxy, alkoxy thioalkoxy, etc.; R6 = Y(:X1)(R4)a, S(O)bR5, acylalkyl, carboalkoxy, cyano, COR8, CO2R8 where R8 = H, alkyl, F; R7 = alkyl; a,n = 1, 2; b = 0, 1, 2], useful as pesticides, are prepd. by reaction of R1(AC:CA1)nC(:O)B (B = leaving group) with MNR2R3 (M = H, metal) or reaction of R1(AC:CA1)nC(:X)NR2R9 (R9 = H, trialkylsilyl) with R3X2 (X2 = leaving group). Treatment of 1 g (EtO)2P(O)NHCH2CHMe2 in THF with 3 mL 1.6 M BuLi/hexane at -60.degree. for 3 h, followed by addn. of 506 .mu.L (2E,4E)-Me(CH:CH)2COCl gave (2E,4E)-II

which showed LD50 of 2 .mu.g against Blatella germanica.

=> ~~l~~yoff hold

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 2.69 | 168.53 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -0.62 | -2.48 |

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:52:36 ON 09 APR 2002

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOG IN ID: sssptal623paz

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 07:46:04 ON 09 APR 2002
FILE 'CAPLUS' ENTERED AT 07:46:04 ON 09 APR 2002
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| | | |
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| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 2.69 | 168.53 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -0.62 | -2.48 |

=> ~~ox~~amflatin

L9 8 OXAMFLATIN

=> dl9 1-8 ti

L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI Structurally simple TSA-like straight chain hydroxamates as potent
histone
deacetylase inhibitors

L9 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI Simple analogs of trichostatin A as potential inhibitors of histone
deacetylase

L9 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI Chemical inducers for morphological reversion of oncogenically
transformed
NIH3T3 cells

L9 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI The novel anti-tumor agent ~~ox~~amflatin differentially regulates
urokinase and plasminogen activator inhibitor type 2 expression and

inhibits urokinase-mediated proteolytic activity

L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI Trichostatin and leptomycin: inhibition of histone deacetylation and signal-dependent nuclear export

L9 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI **Oxamflatin** is a novel antitumor compound that inhibits mammalian histone deacetylase

L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI Inhibitors of Ras-transformation

L9 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI **Oxamflatin**: a novel compound which reverses malignant phenotype to normal one via induction of JunD

=> d 19 1-2 ti fbib abs

L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2002 ACS

TI Structurally simple TSA-like straight chain hydroxamates as potent histone deacetylase inhibitors

AN 2002:190335 CAPLUS

TI Structurally simple TSA-like straight chain hydroxamates as potent histone deacetylase inhibitors

AU Woo, Soon Hyung; Bouchain, Giliane; Frechette, Sylvie; Allan, Martin; Abou-Khalil, Elie; Leit, Silvana; Moradei, Oscar; Vaisburg, Arkadii; Bernstein, Naomy; Fournel, Marielle; Yan, Pu T.; Trachy-Bourget, Marie-Claude; Kalita, Ann; Beaulieu, Carole; Li, Zuomei; Macleod, Robert; Besterman, Jeffrey; Delorme, Daniel

CS Department of Medicinal Chemistry, Methylogene Inc, Montreal, QC, H4S2A1, Can.

SO Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), MEDI-216 Publisher: American Chemical Society, Washington, D. C.
CODEN: 69CKQP

DT Conference; Meeting Abstract

LA English

AB Histone deacetylases (HDACs) are critically important in the functional regulation of gene transcription as well as chromatin structure remodeling

and have become an emerging target in the search for new anticancer drugs.

Several small mol. inhibitors of HDAC, such as the natural product trichostatin A (TSA) and the synthetic compds. suberoylanilide hydroxamic acid (SAHA), and **oxamflatin**, have been reported to induce differentiation of several cancer cell lines and suppress cell proliferation. As part of our efforts to discover novel HDAC inhibitors, we have synthesized a series of structurally simple TSA-like straight chain hydroxamates by varying chain length, aryl substitution, and aryl-chain connection (e.g. ketone, alkene, oxime etc). Some of these compds. inhibit partially purified human HDAC with IC 50 of low nanomolar range, comparable with those of TSA. These compds. induce hyperacetylation of histones at uM concns. and significantly inhibit proliferation in human cancer cells. They can also induce expression of p21, apoptosis, and cell cycle blocks in human cancer cells. In this

presentation we describe synthesis of these new compds. as well as SAR results from enzyme inhibition and cellular potency.

L9 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2002 ACS
TI Simple analogs of trichostatin A as potential inhibitors of histone deacetylase
AN 2002:190334 CAPLUS
TI Simple analogs of trichostatin A as potential inhibitors of histone deacetylase
AU Paul, Brajeswar; Mayer, Bruce F.; Asch, Bonnie; Asch, Harold
CS Grace Cancer Drug Center, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SO Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, United States, April 7-11, 2002 (2002), MEDI-215 Publisher: American Chemical Society, Washington, D. C.
CODEN: 69CKQP
DT Conference; Meeting Abstract
LA English
AB An antibiotic, trichostatin A (TSA), is a potent inhibitor of histone deacetylase (HDAC) and a highly effective inducer of differentiation in several types of cancer cells. Histones are major determinants of chromatin structure, with acetylation playing a key role in how tightly they bind to DNA and thus regulating accessibility of DNA to transcription factors. Several complex natural products: trapoxin, herbimycin, radicicol, depudecin, apicidin, FR 901228 and a few synthetic congeners: SAHA (suberoylanilide hydroxamic acid) and **oxamflatin** have been identified as HDAC inhibitors and reported to revert the morphol. changes following the transformation of cells in culture. We have synthesized a set of simple analogs of TSA in as little as five synthetic steps. These compds. are interesting leads for the design of potent inhibitors of HDAC and development of potential therapeutic agents for chemoprevention and treatment of cancer. Synthesis, phys. and biol. data will be presented. (Supported by NIH Grant CA16056).

=> logoff hold

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 13.53 | 179.37 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| -1.86 | -3.72 |

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STN INTERNATIONAL SESSION SUSPENDED AT 07:49:22 ON 09 APR 2002